Towards Fully Interpretable Deep Neural Networks: Are We There Yet?

Sandareka Wickramanayake\textsuperscript{1} \quad Wynne Hsu\textsuperscript{1,2} \quad Mong Li Lee\textsuperscript{1,2}

\section*{Abstract}

Despite the remarkable performance, Deep Neural Networks (DNNs) behave as black-boxes hindering user trust in Artificial Intelligence (AI) systems. Research on opening black-box DNN can be broadly categorized into post-hoc methods and inherently interpretable DNNs. While many surveys have been conducted on post-hoc interpretation methods, little effort is devoted to inherently interpretable DNNs. This paper provides a review of existing methods to develop DNNs with intrinsic interpretability, with a focus on Convolutional Neural Networks (CNNs). The aim is to understand the current progress towards fully interpretable DNNs that can cater to different interpretation requirements. Finally, we identify gaps in current work and suggest potential research directions.

\section{1. Introduction}

Deep Neural Networks (DNNs) have demonstrated impressive performance in a wide range of tasks such as computer vision (He et al., 2016; Huang et al., 2017; Liu et al., 2016; Tan et al., 2020), natural language processing (Sutskever et al., 2014; Peters et al., 2018), sentiment analysis (Yang et al., 2019; Sachan et al., 2019), etc. Also, applications of DNNs span many domains, including robotics, retail, manufacturing, and even safety-critical domains such as healthcare (Cheng et al., 2016; Che et al., 2016; Litjens et al., 2017). However, DNNs behave as black-boxes where users can neither understand the decision-making procedure nor the reasons behind their predictions. This opaque nature has affected the acceptance and deployment of DNN-based applications.

Research on opening black-box DNNs can be broadly categorized into post-hoc methods and inherently interpretable DNNs. The objective of post-hoc interpretation methods is to provide insights into already trained models. They aim to uncover either the meaning of the learned features (Bau et al., 2017; Olah et al., 2018) or the rationale behind the model decisions (Zeiler & Fergus, 2014; Bach et al., 2015; Hendricks et al., 2016; Selvaraju et al., 2017; Park et al., 2018; Olah et al., 2018; Ghorbani et al., 2019; Yeh et al., 2019; Kim et al., 2017; 2018; Wickramanayake et al., 2019). These post-hoc methods can be applied without changing the underline model or retraining it. On the other hand, inherently interpretable DNNs require architectural changes or regularizations to provide intrinsic explanations (Li et al., 2018; Melis & Jaakkola, 2018; Chen et al., 2019a; Wickramanayake et al., 2021). Table 1 gives a summary of the pros and cons of these two categories.

In this paper, we review existing interpretable DNNs, with a focus on CNNs, namely DNNs with in-built attention (Zhang et al., 2014; Zheng et al., 2017; Zhou et al., 2018; 2016; Pillai & Pirsiavash, 2021), DNNs with prototype-based reasoning (Li et al., 2018; Melis & Jaakkola, 2018; Chen et al., 2019a) and DNNs with feature regularizations (Zhang et al., 2018; Huang & Li, 2020; Liang et al., 2020; Wickramanayake et al., 2021).

\section{2. DNNs with in-built Attention}

Integrating attention to DNNs is a common approach for natural language processing (Martins & Astudillo, 2016; Wang et al., 2016), domain-specific interpretable DNNs (Chen et al., 2019c; Gao et al., 2018) and fine-grained image classification tasks (Zeng et al., 2017; Fu et al., 2017; Zhuang et al., 2020). These models aim to expose the parts of an input the model focuses on for decision making.

Multi-Attention CNN (MA-CNN) (Zheng et al., 2017) consists of convolution, channel grouping, and classification sub-networks. Given an input image, MA-CNN feeds the image through a set of convolutional layers and extracts feature maps. Feature maps are then passed to a channel grouping network to obtain multiple attention areas. These attention areas are used to classify the input image. Visualizations of attention maps show that MA-CNN focuses on diverse image areas with strong discrimination ability.

Recurrent-Attention CNN (RA-CNN) (Fu et al., 2017)
uses an attention proposal sub-network to locate the discriminative areas. It then scales the discriminative areas to examine the details in these areas. Such attention localization at different scales helps to identify class specific regions.

Class Activation Map (CAM) (Zhou et al., 2016) builds attention-based interpretability into standard CNNs. This method replaces the fully connected (FC) layers with a Global Average Pooling (GAP) layer. Saliency maps with respect to a class $c$ are generated by multiplying each feature map in the final convolutional layer with its weight corresponding to $c$ and taking the channel-wise summation. The resultant saliency map indicates the image regions the model has focused on to classify the given image to $c$.

CI-GC (Pillai & Pirsiavash, 2021) is a self-supervise learning approach to encourage the model to learn consistent interpretations given an explanation mechanism such as saliency map. A new image is created whereby an input image is placed on a random cell in a $2 \times 2$ grid, and other three cells are filled with images selected from classes different from that of the input image. The model is trained to minimize the difference between the saliency map of the newly created image and its targeted interpretation, in addition to maximizing the log-likelihood of the correct class. The targeted interpretation is obtained by placing the saliency map of the input image in the corresponding cell and setting the attribution values in other quadrants to zero.

### 3. DNNs with Prototype-based Reasoning

PrototypeDNN proposed in (Li et al., 2018) trains a convolutional auto-encoder to learn a set of prototypes and a prototype classification network to produce the probability distribution over the classes. Model decisions are explained by presenting decision-relevant prototypes visualized using the decoder.

(Melis & Jaakkola, 2018) propose a Self-Explainable Neural Network (SENN), which is a generalized version of (Li et al., 2018). SENN consists of three networks: (a) a concept encoder to generate interpretable concepts, (b) an input-dependent parameterizer to generate relevance scores of those concepts, and (c) a linear aggregator to combine concepts-relevance score pairs to derive the decision. The interpretable concepts can be obtained from expert knowledge or automatically learned with three desiderata:

- **Fidelity** - learned concepts capture relevant information about the input;
- **Diversity** - learned concepts have minimum overlap;
- **Grounding** - learned concepts are human understandable.

ProtoPNet (Chen et al., 2019a) adds a new prototype layer and learns a pre-determined number of prototypes for each class $c$. The learning objective is designed to ensure that the set of prototypes for class $c$ captures the most relevant concepts for identifying images of that class. In the inference phase, ProtoPNet compares the latent features of an input image against learned prototypes to evaluate if the input image is from class $c$. The comparison is carried by calculating Euclidean distances between each prototype and all the patches of the latent features that have the same shape as the prototype and inverts the distances into similarity scores. The maximum of these similarity scores indicates how strongly a prototype is present in some patch of the input image. The maximum scores of all the prototypes are multiplied by the weight matrix of class $c$ to give the final score that the input image belongs to $c$.

### 4. DNNs with Feature Regularization

InterpCNN (Zhang et al., 2018) introduces a new loss function to encourage each conv-filter in the higher level convolution layers to be activated only for a specific object part. This loss function maximizes the mutual information between the conv-filter’s feature map and a template. A template is the ideal distribution of activations for the feature map given an image. If the given image is from category $c$, a single location of the feature map should be activated. Otherwise, the feature map should remain inactivated. The training uses image-level labels without the need for object part-level annotations. The filter loss pushes the feature map of a conv-filer towards representing a specific object part during the learning process.

Region-CNN (Huang & Li, 2020) is an interpretable classifier specific for fine-grained recognition. It learns to group pixels into meaningful object part regions by enforcing a prior distribution for the occurrence of each part.
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Table 2. Categorization of interpretable DNNs based on the type of explanations.

| Type of explanation | Methods |
|---------------------|---------|
| Saliency maps       | MA-CNN (Zheng et al., 2017), RA-CNN (Fu et al., 2017), CAM (Zhou et al., 2016), Region-CNN (Huang & Li, 2020), CI-GC (Pillai & Pirsiavash, 2021) |
| Prototypes          | PrototypeDNN (Li et al., 2018), SENN (Melis & Jaakkola, 2018), ProtoPNet (Chen et al., 2019a) |
| Word phrases        | CCNN (Wickramanayake et al., 2021) |

CCNN (Wickramanayake et al., 2021) adds an additional concept layer to a CNN-based architecture to guide the learning of the associations between visual features and word phrases extracted from image descriptions. The training objective function takes into consideration concept uniqueness and mapping consistency. The former encourages each learned concept to correspond to only one word phrase, while the latter aims to preserve the distance between the learned concept and its corresponding word phrase in a joint embedding space. Together with classification accuracy loss, this training objective ensures that CCNN is both accurate and interpretable. CCNN employs a GAP layer to reduce the dimensionality of the concept layer’s outputs before feeding to a fully connected layer. Hence, CCNN classification decisions can be expressed as a weighted sum of the learned concepts. In other words, CCNN can explain its decisions in terms of word phrases and their corresponding contributions.

5. Discussion

We observe that most of the interpretable DNNs described in the previous section make decisions based on a linear aggregation of the learned interpretable features. The difference lies in how the interpretable features are defined and how such features are learned. For example, InterpCNN uses disentangled concepts, ProtoPNet and SENN use prototypes and CCNN uses features that correspond to word phrases. Figure 1 shows the features learned by CCNN, ProtoPNet, CI-GC, InterpCNN and CAM taken from (Wickramanayake et al., 2021). We see that some of these features may not correspond to concepts consistent with human perception. For instance, although InterpCNN (Zhang et al., 2018) strives to learn features that correspond to high-level concepts, the learned features cover only part of the region when the concept spans multiple non-contiguous regions in the image, e.g., when an image of two cats is given, the filter has activated for the chest of only one cat.

Another observation is that these interpretable DNNs differ in the type of explanations they provide, from saliency maps to prototypes to word phrases (see Table 2). We see that CCNN is the only one offering explanations in the form of word phrases. Further, many of these interpretable models can only explain an individual data point’s prediction, whereas ProtoPNet and CCNN can additionally provide the concepts important for predicting a certain class. For example, ProtoPNet can show the prototypes that contribute to the highest number of correct classifications of a class, while CCNN can give the word phrases corresponding to the set of visual features that is activated by the largest number of images in the class.

We also notice inconsistencies among the evaluation studies in existing work. While interpretable DNNs should be evaluated for both predictive performance and interpretability, some of the current work have neglected either of aspects, e.g., SENN is not assessed for classification accuracy whereas ProtoPNet is not quantitatively evaluated for its interpretability. Further, although it is intuitive that explanations intrinsic to the model are more faithful than post-hoc explanations, systematic evaluations should
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be provided to convince the user. Currently, only (Melis & Jaakkola, 2018) conduct experiments to evaluate the faithfulness of generated explanations to the model decision.

6. Conclusion and Future Research

Regardless of how interpretable DNNs generate their explanations, we believe that there is a need to cater to different users who may want to understand the DNNs from different perspectives. For instance, one might be interested in understanding the rationale behind a specific decision of the model, while another wants to know what concepts are used by the model to differentiate a given class. Another user might be keen to understand what changes in the input would change the model prediction to a pre-defined output. Ideally, a fully interpretable system should be able to provide all these explanations, which none of the existing interpretable DNNs are able to. Investigating ways to provide explanations from multiple perspectives is a promising research direction.

Another direction is to have a unified criterion to evaluate interpretability of learned features. Existing work have introduced various metrics such as part interpretability and location instability (Zhang et al., 2018), homogeneity and single-ness (Wickramanayake et al., 2021). The first three metrics indicate if a conv-filter is activated for the same concept across multiple images, while the last metric single-ness indicates if a conv-filter is activated for a unique concept in a given image. We believe that the notion of an interpretable feature being ill-defined has led to numerous metrics. Given that feature interpretability is an essence of a fully interpretable DNN, having a unified objective metric to evaluate feature interpretability would enable researchers to benchmark different inherently interpretable DNNs.

Finally, developing interpretable DNNs that provide semantic explanations is another promising research direction. We see that most explanations provided by current interpretable DNNs are visual explanations, either in the form of saliency maps or prototypes. However, visual explanations may be ambiguous and the ability to explain DNN decisions using semantic concepts are more useful (Wickramanayake et al., 2019; Chen et al., 2019b). The work in (Wickramanayake et al., 2021) has taken the first step in this direction by using image descriptions to learn visual concepts that are consistent with human-understandable concepts.

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