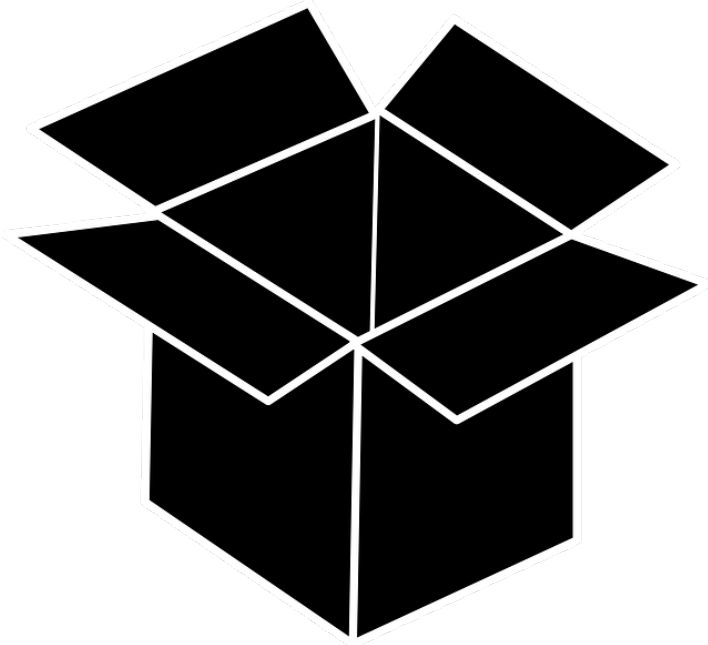
Interpretable Machine Learning

Fundamental Terms and Concepts



Learning goals

- What is interpretable machine learning (IML) and Explainable Artificial Intelligence (XAI)?
- What is interpretability?
- What is the purpose of IML?
- What are the fundamental terms and concepts of IML?

WHAT IS INTERPRETABLE MACHINE LEARNING

- Machine learning (ML) algorithms algorithmically train predictive models with no or little pre-specifications and assumptions about the data.

- Several algorithms such as decision tree learning create interpretable models. However, most algorithms create models which can be considered a black box.

- We use the term black box, although the internal workings of the model are in fact accessible, but too complex for the human mind to comprehend.

- Interpretable machine learning (IML) is an umbrella term for all models and methods that allow for some kind of interpretation.

WHAT IS EXPLAINABLE AI

- IML is often used synonymously with Explainable AI (XAI). There is no unified standard for these terminologies. We find that XAI often is specifically concerned with the interpretation of neural networks, whereas IML is used as an encompassing term for everything related to model interpretability, i.e., interpretable models such as generalized additive models, model-agnostic techniques, as well as interpretations of neural networks.

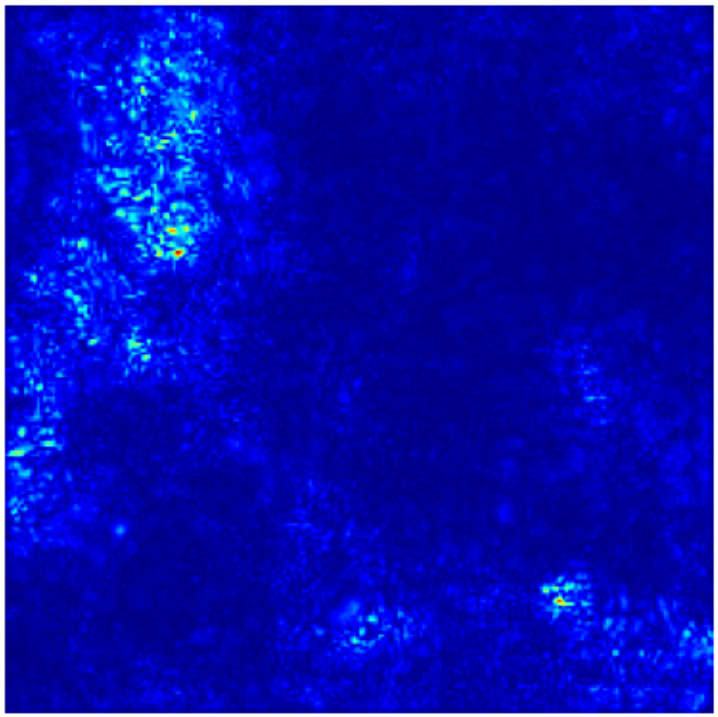
- The nature of neural networks allows for powerful model-specific interpretation techniques, e.g., layer-wise relevance propagation (LRP) and saliency maps. They have in common that influence on the output layer is backpropagated through the entire network layer by layer up to the input layer.

XAI - SALIENCY MAPS

- The traditional assumption is that deep learning is best suited for non-tabular data, whereas other ML techniques such as gradient boosting or random forests are better suited for tabular data. However, recent developments seem to undermine this assumption, i.e., neural networks increasingly outperform other methods on tabular data as well.

- For visual data, i.e., pixels being represented as a matrix, deep learning has proven to deliver remarkable results. The default way to interpret neural networks on visual data is a saliency map. A saliency map is a heatmap indicating pixel influence on the prediction (e.g., a classification of an image):

XAI - SALIENCY MAPS



WHAT IS INTERPRETABILITY?

- There is no scientific consensus on the definition of interpretability.
- We need to differentiate between interpretations of a model or reality. The latter is distorted by all modeling fallacies involved in predictive modeling, e.g., data quality, under- and overfitting, or model extrapolations.
- For practical purposes, we decide to define interpretability such that it is beneficial to our modeling tasks. Think back to the foundations of statistical modeling: the linear regression model (LM). The LM, with its known equation of beta coefficients, represents a paradigm for statistical interpretability.
- It follows that it would be beneficial to create techniques that give us an interpretation similar to the one of an LM.

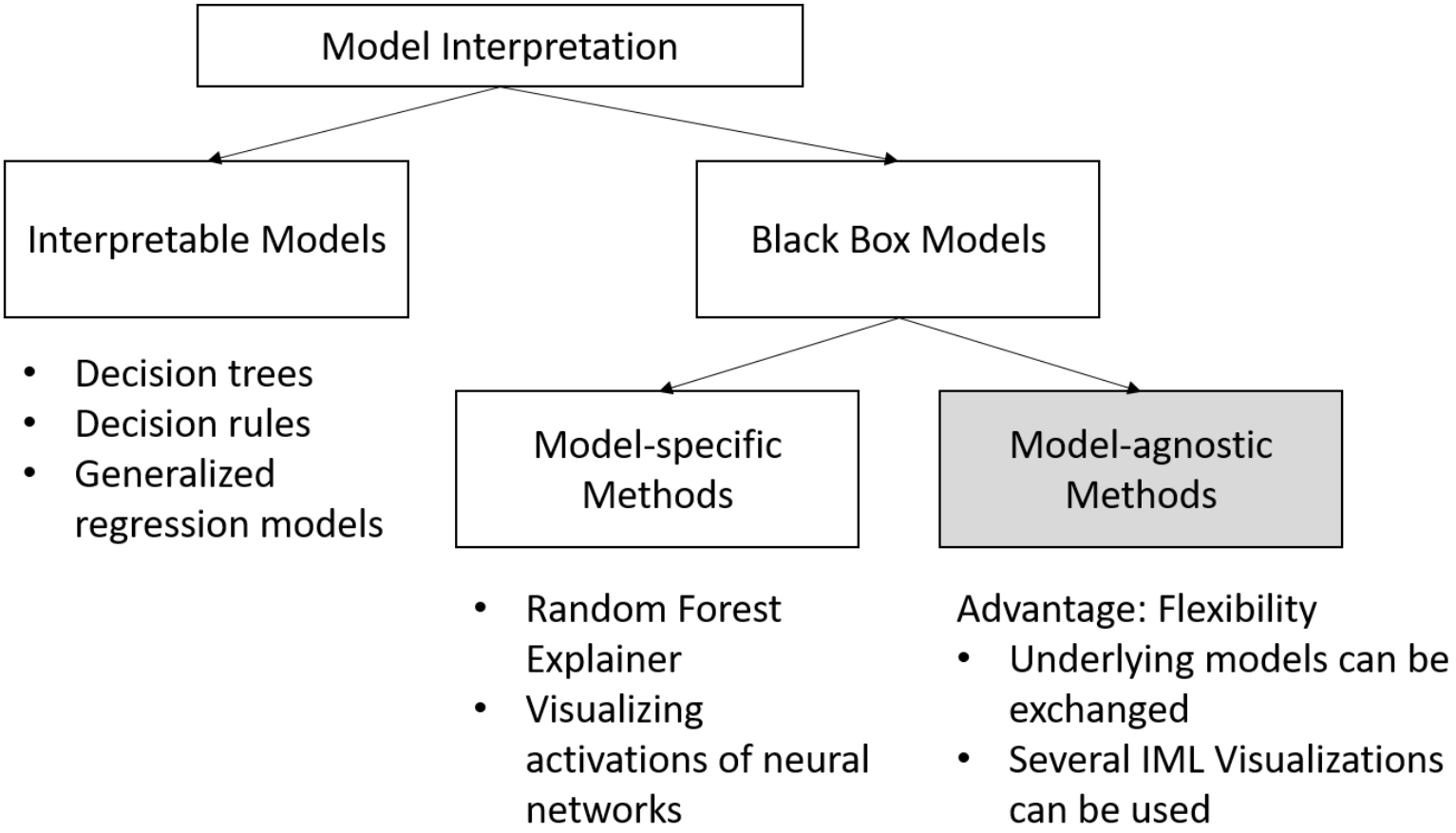
FUNDAMENTAL TERMS AND CONCEPTS

- **Feature effects and importance:** An effect indicates the direction and magnitude of a change in predicted outcome due to changes in feature values. The importance indicates the contribution of one or multiple features to the model performance, or variance in predicted outcome.

- **Local and global:** A local interpretation is an interpretation for a single observation, or data instance, i.e., a single location in multidimensional feature space. A global interpretation is an interpretation for the entire feature space. Furthermore, increasing emphasis is put on semi-global interpretations, which are interpretations on feature subspaces.

- **Model-specific and model-agnostic:** A model-specific method is tied to the use of a specific model. A model-agnostic one can be applied to any predictive model.

WHAT TOOLS DO WE HAVE?



$\Rightarrow$ Due to their versatility, both industry and academia put a large focus on model-agnostic methods, which we will focus on!

CORRELATION VERSUS INTERACTION

- You will discover that a lot of problems in IML arise due to correlated features and feature interactions. One needs to be careful not to confuse them.

- Correlated features imply that the joint probability density function (PDF) between features is not a product of their marginal distributions, i.e., $\mathcal{F}(x_1, \ldots, x_p) \neq \mathcal{F}(x_1) \cdot \ldots \cdot \mathcal{F}(x_p)$. This becomes a problem when interpretation methods rely on model evaluations in artifically sampled data points which may be located in areas where the model extrapolates if the training data is correlated.

CORRELATION VERSUS INTERACTION

- An interaction is a product term between features inside the prediction function. As such, interactions are detached from the constitution of the data, i.e., regardloss of the degree of correlation, the effect of a feature on the target will depend on the values of one or multiple other features.