

Interpretable Machine Learning

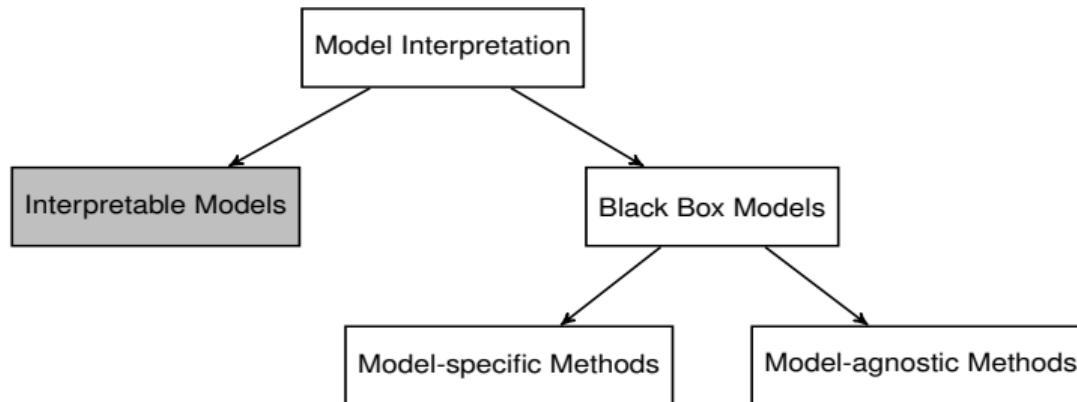
Dimensions of Interpretability



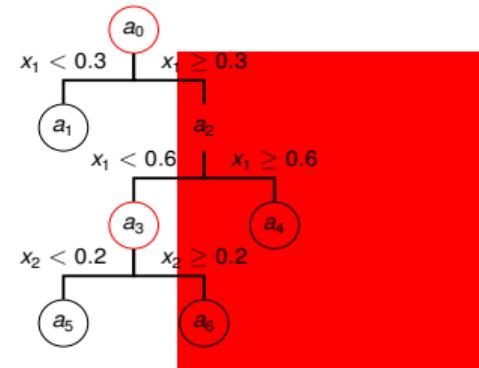
Learning goals

- Intrinsic vs. model-agnostic methods
- Different types of explanations
- Local vs. global methods
- Model or learner explanations – with or without refits
- Levels of interpretability

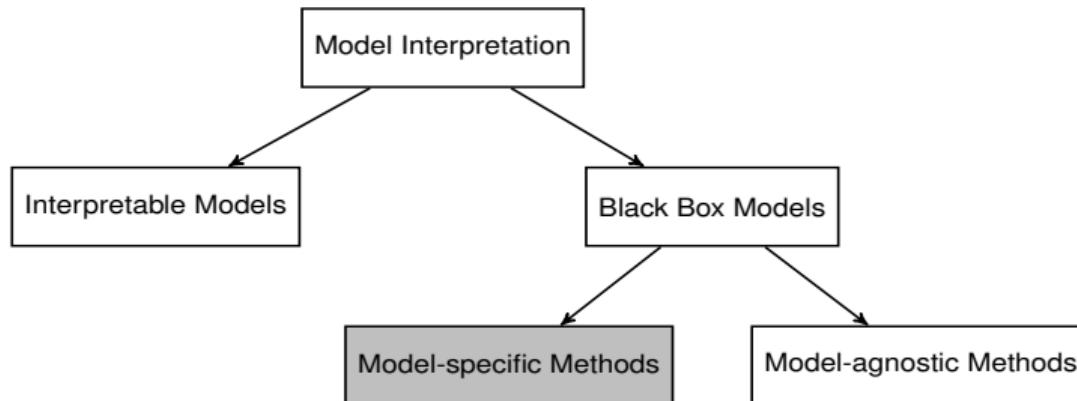
INTRINSIC VS. MODEL-AGNOSTIC



- Intrinsically interpretable models:
 - Examples: linear model, decision tree, decision rule, GLMs
 - Interpretable because of simple model structure, e.g., weighted combination of feature values or tree structure
 - Difficult to interpret with many features / complex interactions

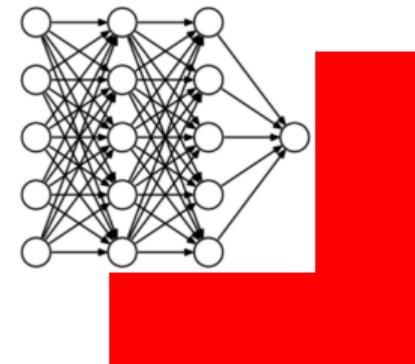


INTRINSIC VS. MODEL-AGNOSTIC

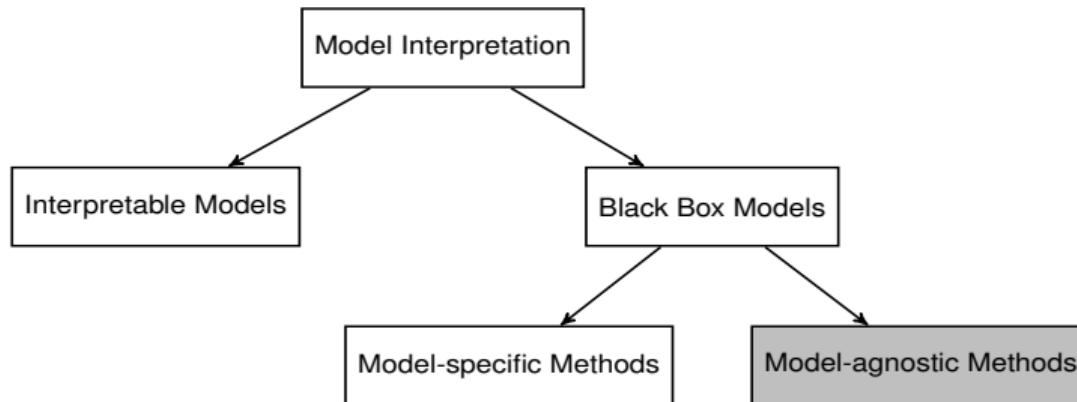


- Model-specific methods:

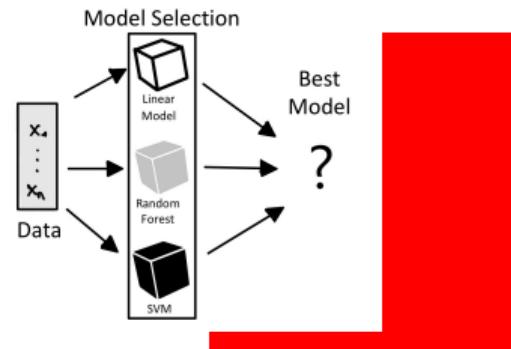
- Interpretation method being applicable to a particular ML model
- Example: implicitly integrated feature interpretation methods in tree based models, e.g., Gini Importance
- Advantage: Can exploit model structure
- Visualize activations of NNs



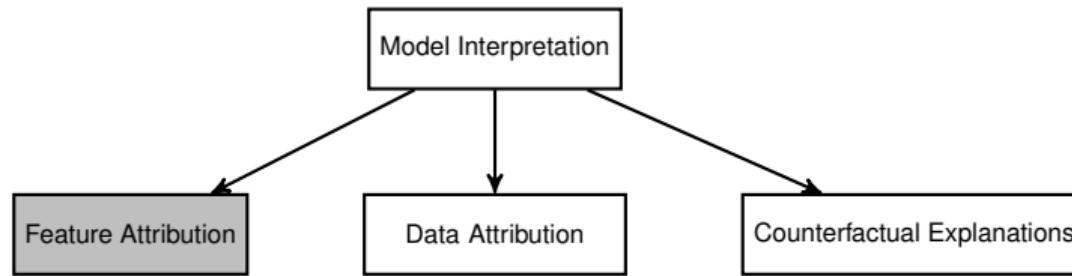
INTRINSIC VS. MODEL-AGNOSTIC



- Model-agnostic methods:
 - In ML: Tune over many model classes
 - ~~ Unknown which model is best / deployed
 - ~~ Need for interpretation methods applicable to any model
 - Applied after training (post-hoc)
 - Applicable to intrinsically interpretable models
 - ~~ provides insights into other types of explanations



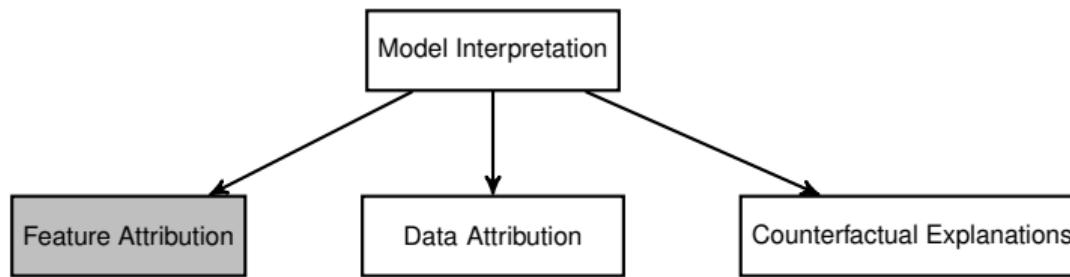
TYPES OF EXPLANATIONS



- Feature Attribution:

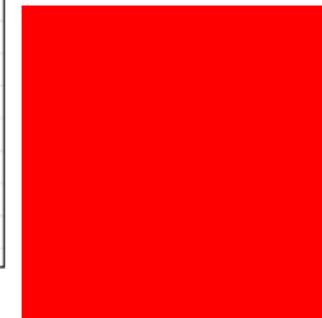
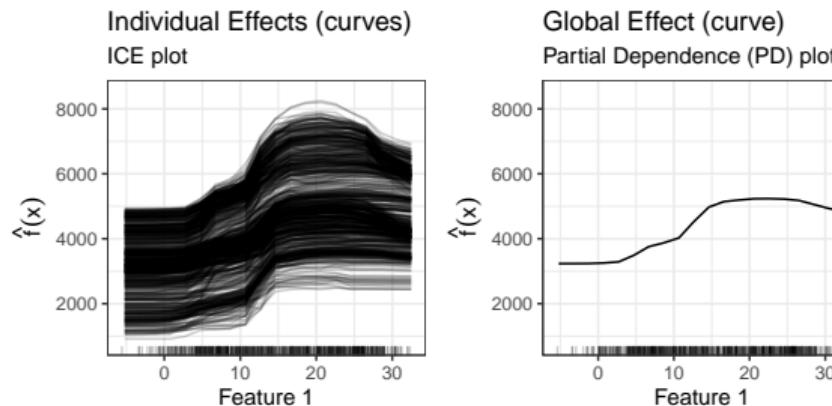
- Produce explanations on a per-feature level, e.g., feature effects or feature importance
 - ~~ Vary feat. values, inspect change of model prediction, model variance or model error

TYPES OF EXPLANATIONS

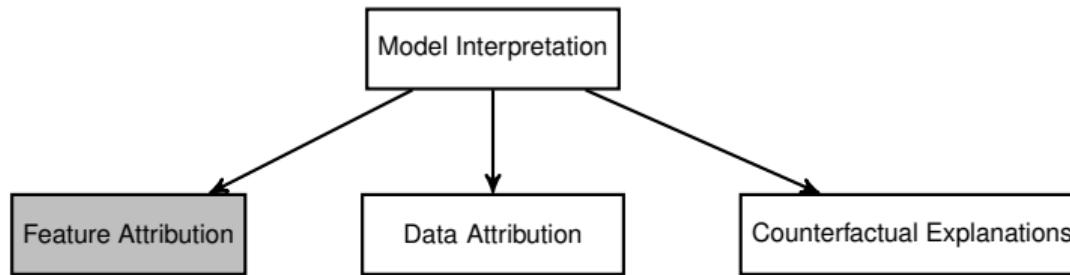


Feature Effects indicate the change in prediction due to changes in feature values.

- Model-agnostic methods:
ICE curves, PD plots ...
- Pendant in linear models:
Regression coefficient θ_j
- Further examples: Saliency
Maps, model-agnostic
methods such as SHAP and
LIME

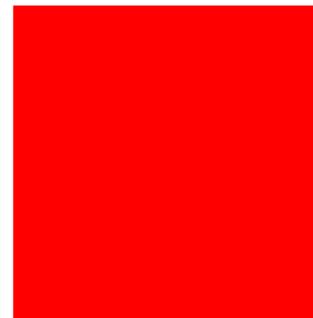
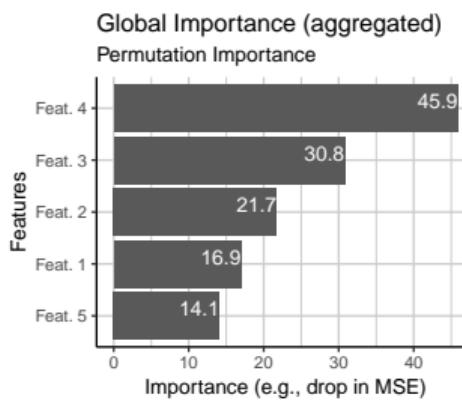


TYPES OF EXPLANATIONS

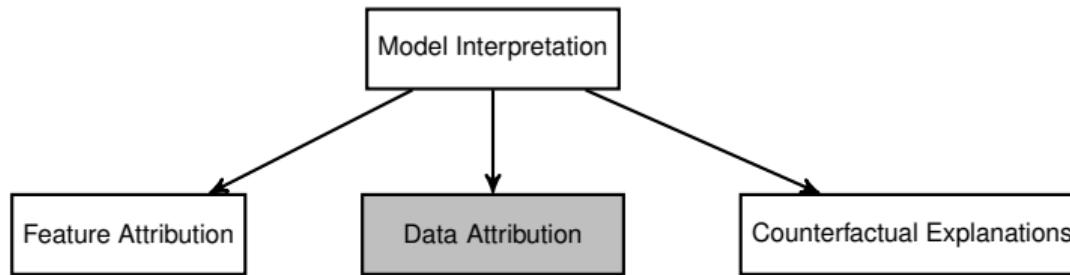


Feature importance methods rank features by how much they contribute to the predictive performance or prediction variance of the model.

- Model-agnostic methods: PFI, ...
- Pendant in linear models: t-statistic, p-value (significant effect)

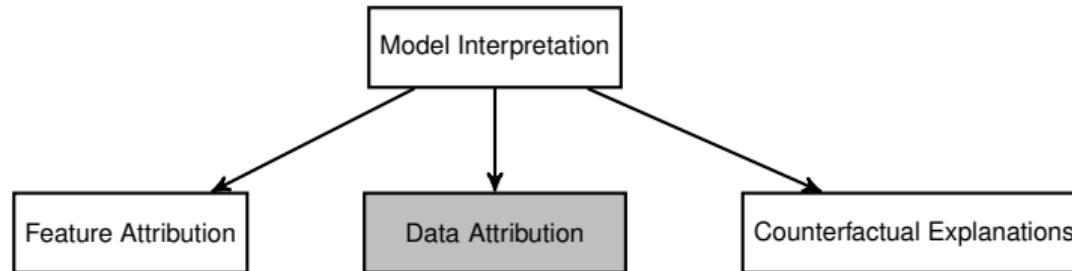


TYPES OF EXPLANATIONS



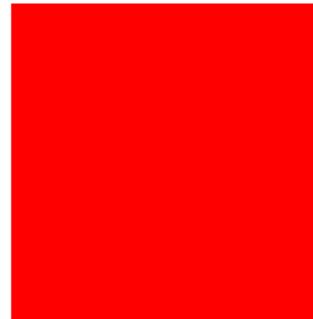
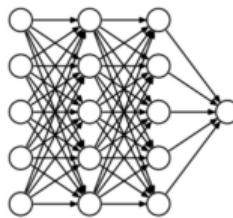
Data Attribution: Identify training instances most responsible for a decision (e.g. Influence Functions)

TYPES OF EXPLANATIONS



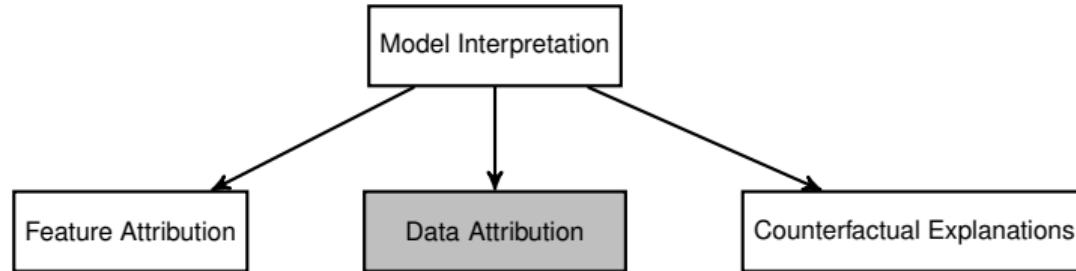
Data Attribution: Identify training instances most responsible for a decision (e.g. Influence Functions)

Example: Consider a model which should distinguish muffins and dogs



How does this incorrect prediction come about?

TYPES OF EXPLANATIONS



Data Attribution: Identify training instances most responsible for a decision (e.g. Influence Functions)

Look at the training data set: Which of the training data points caused the model prediction?

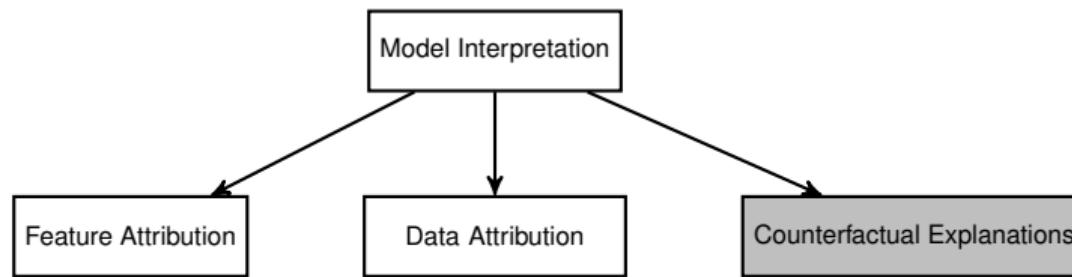


Method searches for the most similar images and bases the decision on them

- ~~ The training images that look most like the new input represent a muffin
- ~~ Wrong output (muffin instead of dog)

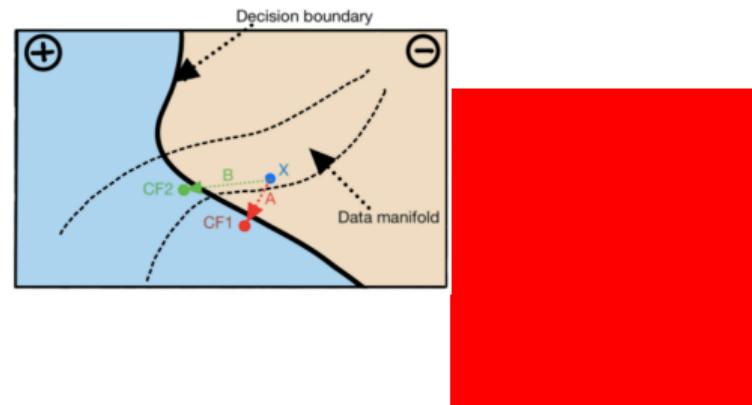


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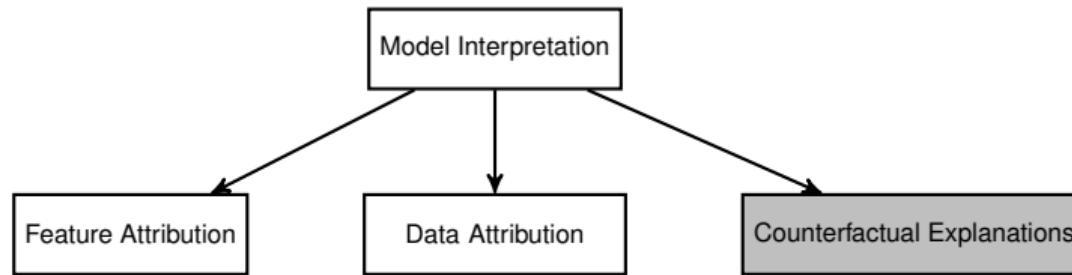


- Counterfactual Explanations:

- Identify smallest necessary change in feature values so that a desired outcome is predicted
- Contrastive explanations
- Diverse counterfactuals
- Feasible & actionable explanations



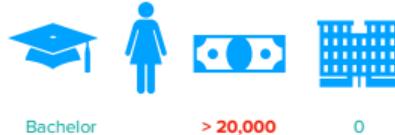
TYPES OF EXPLANATIONS



Example (loan application):



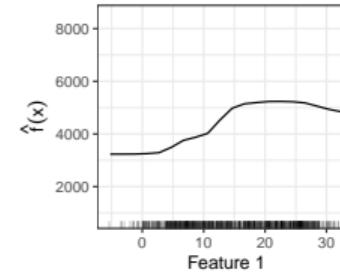
What can a person do to obtain a favorable prediction from a given model ?



GLOBAL VS. LOCAL

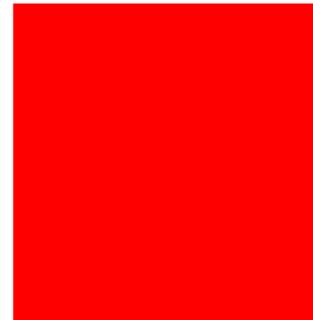
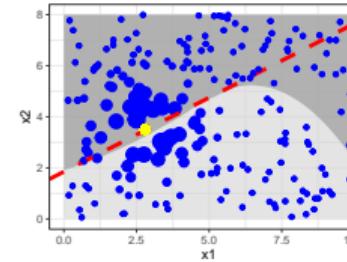
Global interpretation methods explain the model behavior for the entire input space by considering all available observations:

- Permutation Feature Importance (PFI)
- Partial Dependence (PD) plots
- Accumulated Local Effect (ALE) plots
- ...



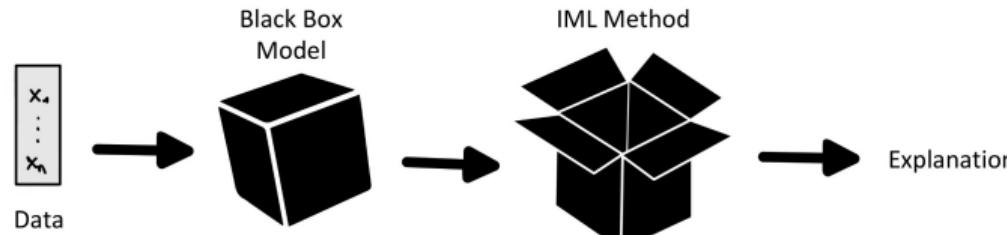
Local interpretation methods explain the model behavior for single data instances:

- Individual Conditional Expectation (ICE) curves
- Local Interpretable Model-Agnostic Explanations (LIME)
- Shapley values, SHAP
- ...



FIXED MODEL VS. REFITS

- Global interpretation methods use a model and data as input and produce explanations
→ Explanations can be viewed as statistical estimators



- Situation in ML: Deployed model is trained on all available data
 - No unseen test data left to, e.g., reliably estimate performance
 - IML method could use the same data the model was trained on to produce explanations
 - But: Some IML methods rely on measuring loss which requires unseen test data
- Alternative: Explain the inducer that created the model (instead of a fixed model)
 - Idea: Use resampling strategies (e.g., 4-fold CV) as in performance estimation
 - Requires refitting

LEVELS OF INTERPRETABILITY

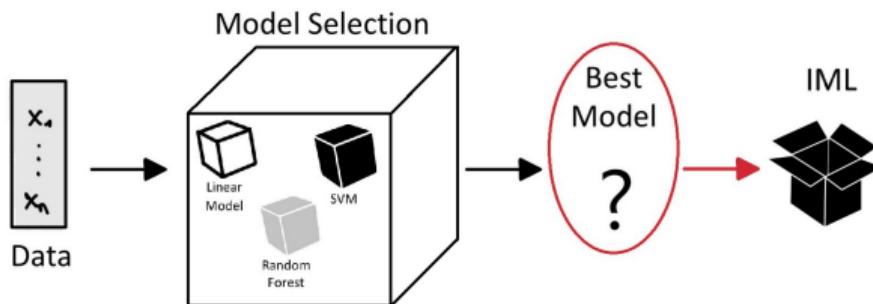
1st
level
view

Research Question

How to explain a given model
fitted on a data set?

Objects of analysis

(deployed) model
 $\theta \mapsto \hat{f}(\theta)$



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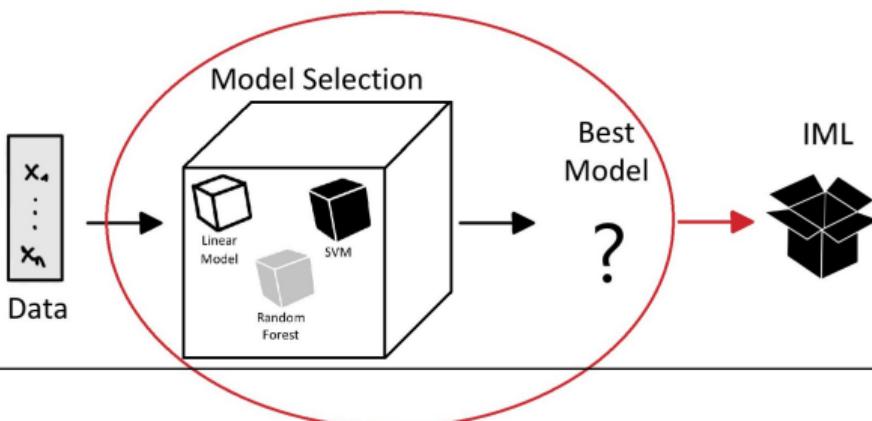
2nd
level
view

How does an optimizer choose a
model based on a data set?

Objects of analysis

(deployed) model
 $\theta \mapsto \hat{f}(\theta)$

Model selection (decisions made
by AutoML systems,
hyperparameter optimization
process, ...)



LEVELS OF INTERPRETABILITY

1st
level
view

Research Question

How to explain a given model fitted on a data set?

2nd
level
view

How does an optimizer choose a model based on a data set?

3rd
level
view

How do properties of data sets relate to performance of a learner and its hyperparameters?

Objects of analysis

(deployed) model
 $\theta \mapsto \hat{f}(\theta)$

Model selection (decisions made by AutoML systems, hyperparameter optimization process, ...)

properties of ML algorithms in general (benchmark)

