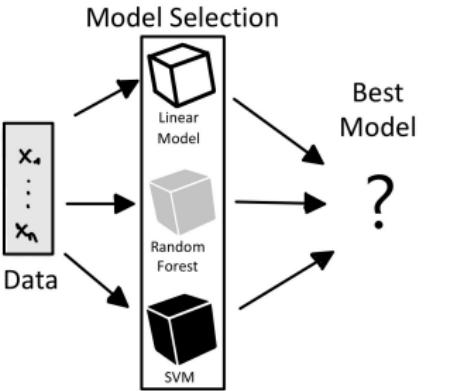


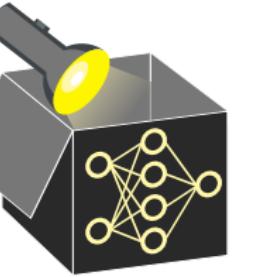
Interpretable Machine Learning

Dimensions of Interpretability



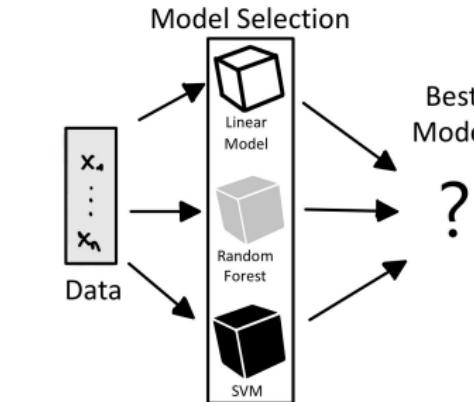
Learning goals

- Difference between intrinsic, model-specific, and model-agnostic interpretability
- Different types of explanations
- Local, global, and regional explanations
- Model/learner explanation (without/with refits)
- Levels of interpretability



Interpretable Machine Learning

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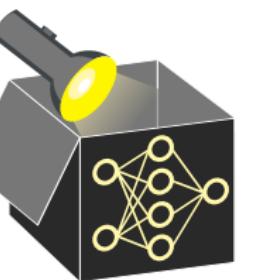
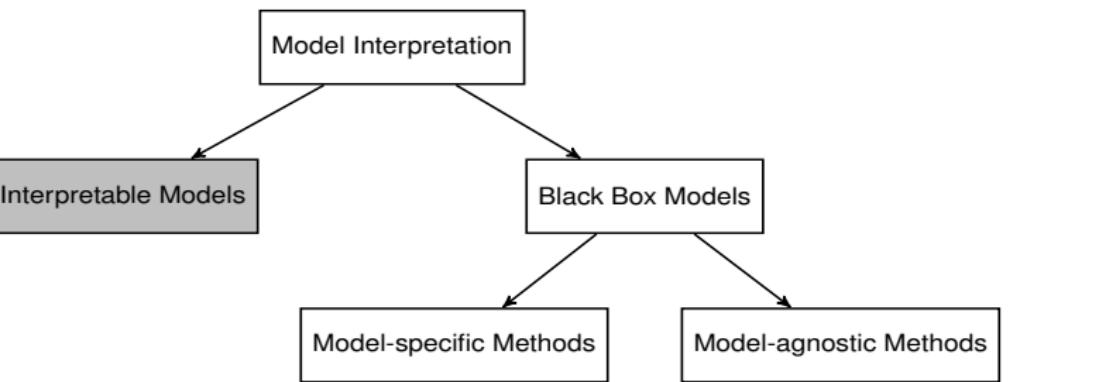


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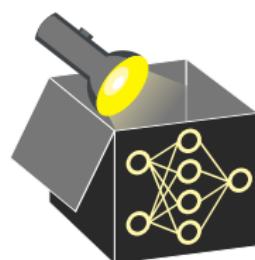
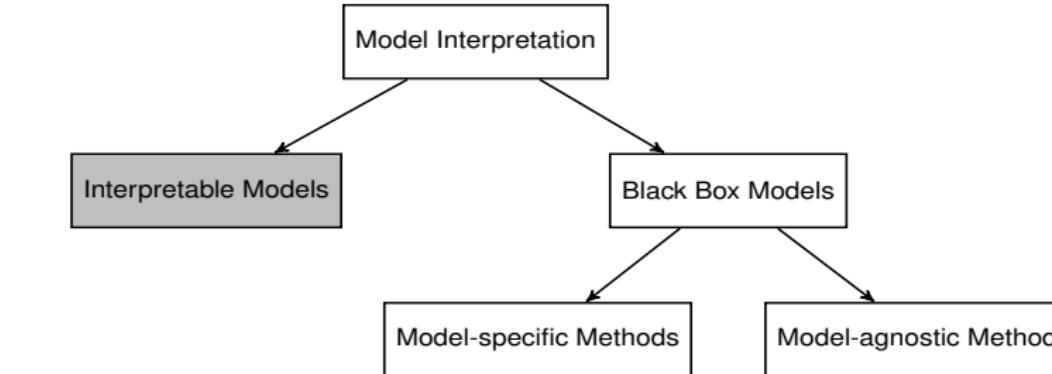
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INTRINSIC, MODEL-SPECIFIC, MODEL-AGNOSTIC

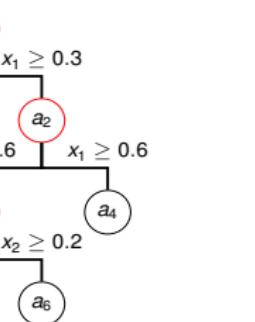


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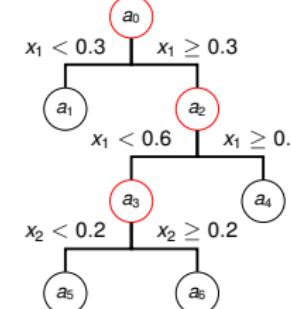
Intrinsically Interpretable Models:

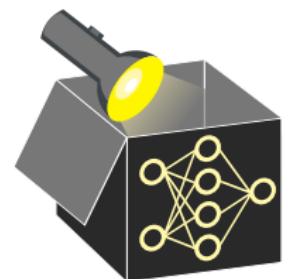
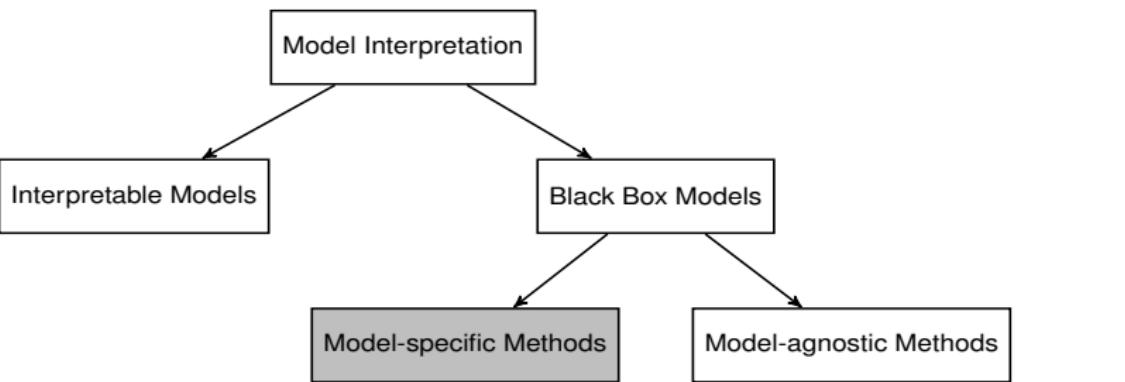
- Simple model structure (e.g., weighted sum or tree)
- Examples: GLMs, decision trees
- Pro: Additional IML methods not necessarily required
- Con: Limited model complexity can reduce performance; can still be hard to interpret with many features /interactions



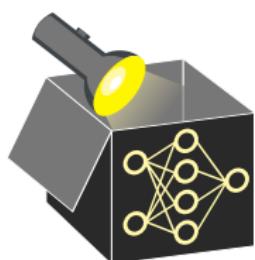
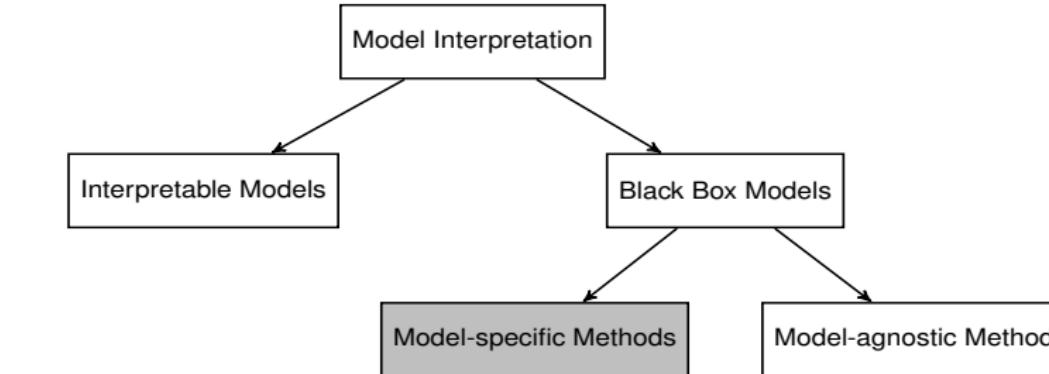
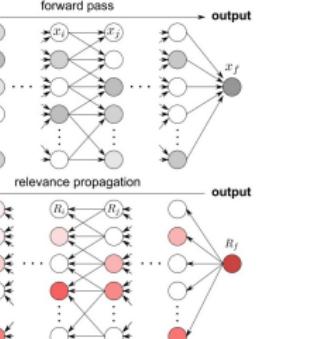
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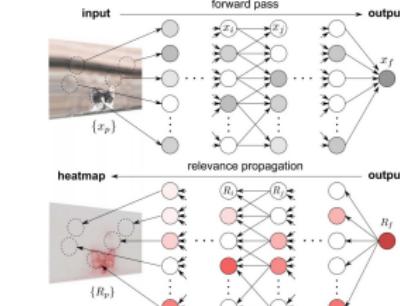


**Model-specific Methods:**

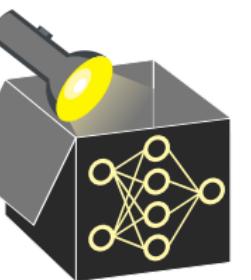
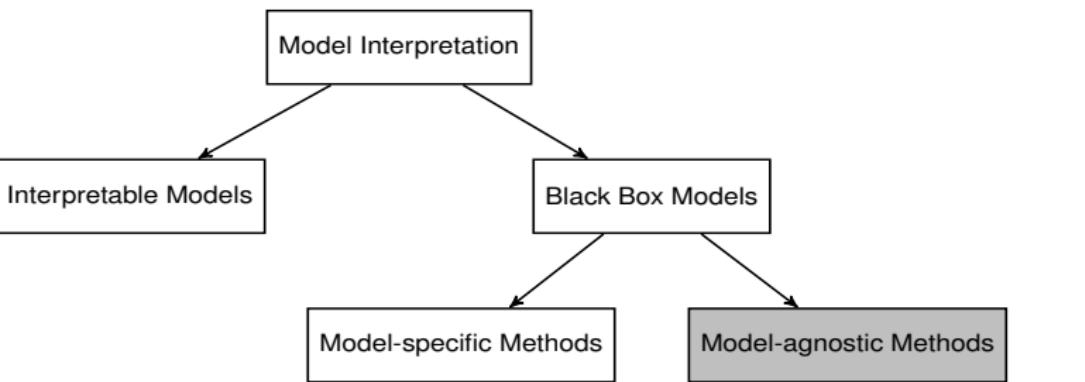
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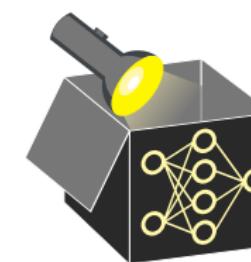
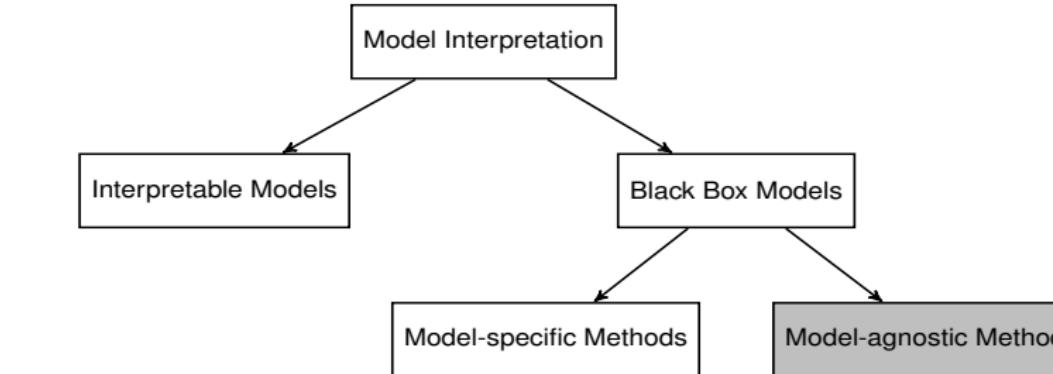
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INTRINSIC, MODEL-SPECIFIC, MODEL-AGNOSTIC

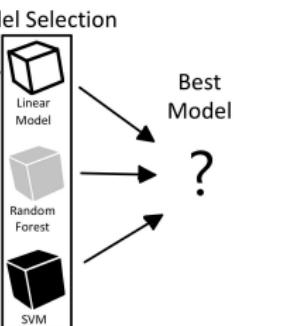


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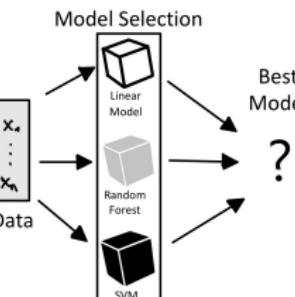
Model-agnostic Methods:

- In ML: Tune over many model classes
 - ~~ Unknown which model is best / deployed
 - ~~ Need for IML methods that work for any model
- Applied after training (post-hoc)
- Applicable to intrinsically interpretable models
 - ~~ provides insights into explanations

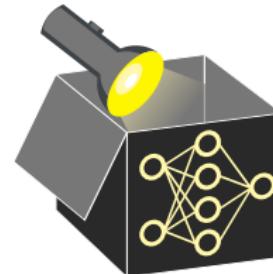
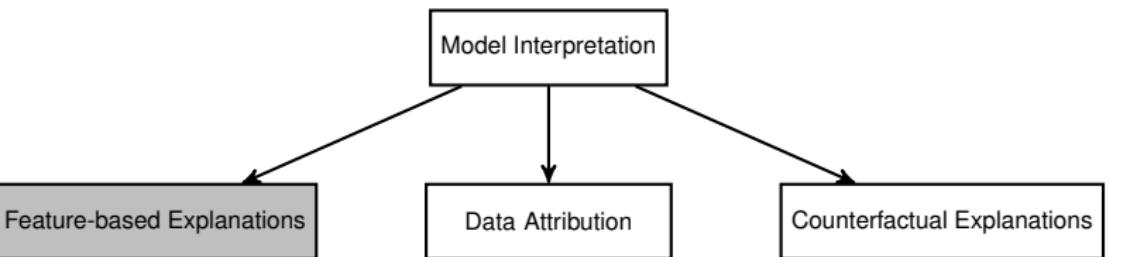


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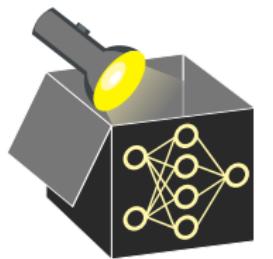
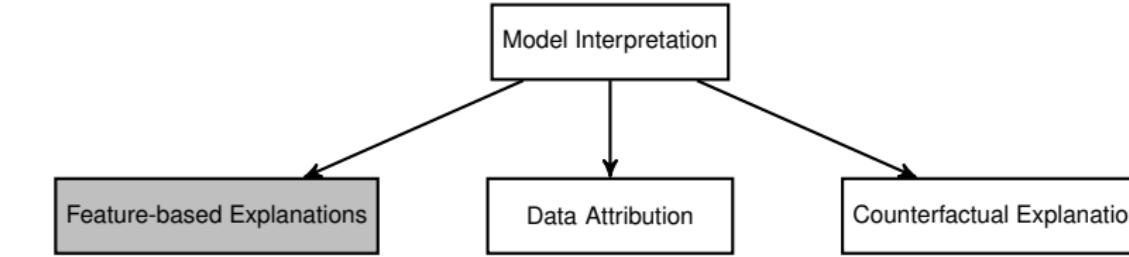
TYPES OF EXPLANATIONS



Feature-based Explanations:

- Analyze the role of individual features in model behavior.
- Types of feature-based explanations:
 - Feature Importance
 - Feature Effects
 - Feature Interactions
- Common principle: Vary or perturb feature values and observe changes in predictions, variance, or performance.

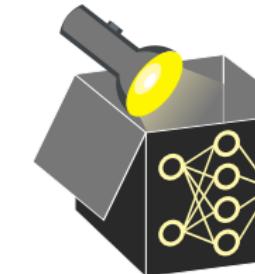
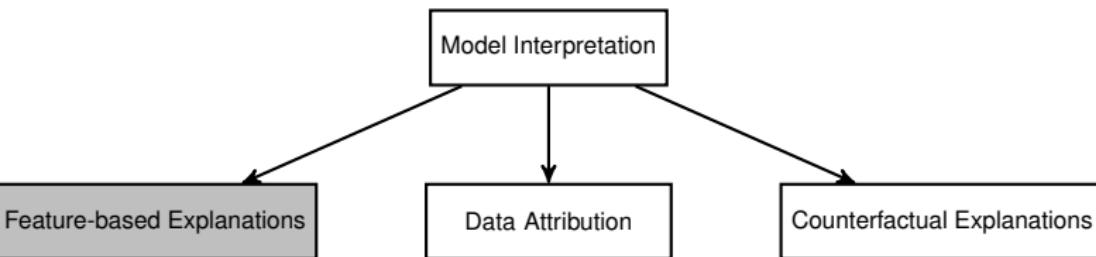
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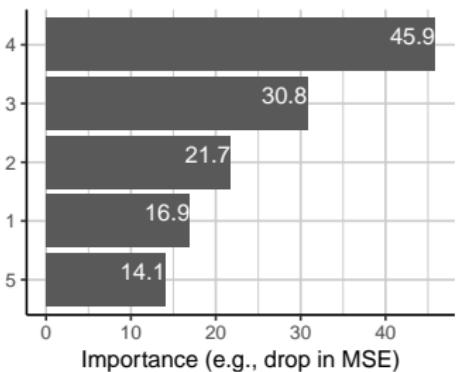
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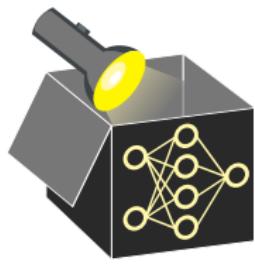
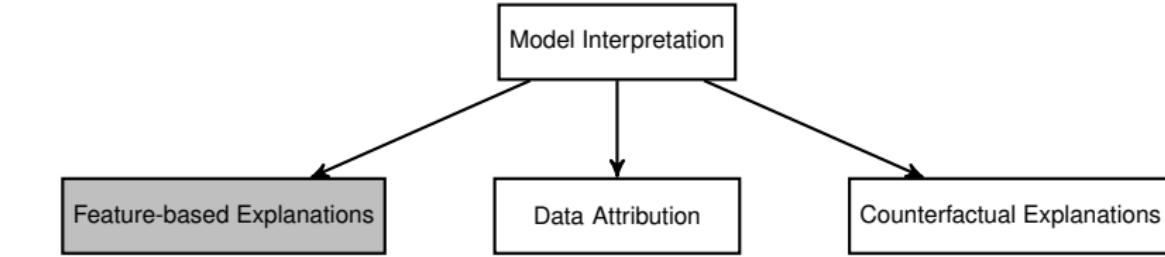


Feature Importance quantifies relevance of features, e.g., their contribution to model prediction, predictive performance, or prediction variance.

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

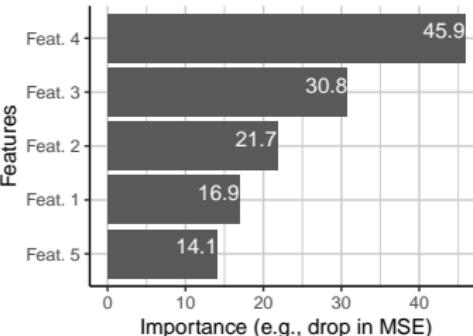


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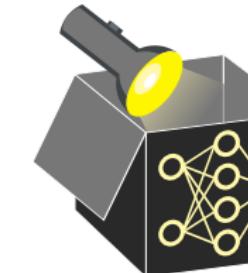
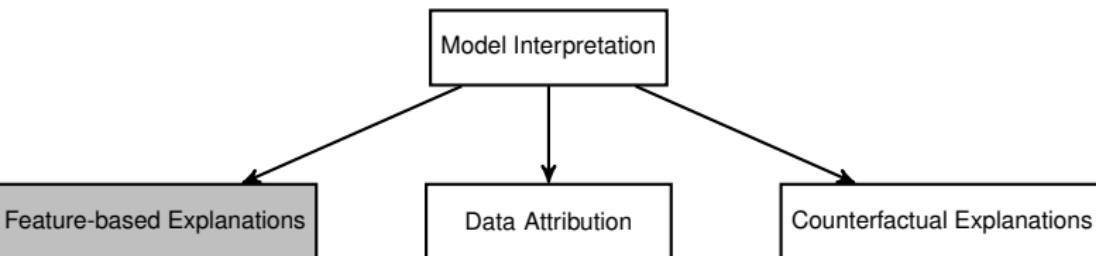


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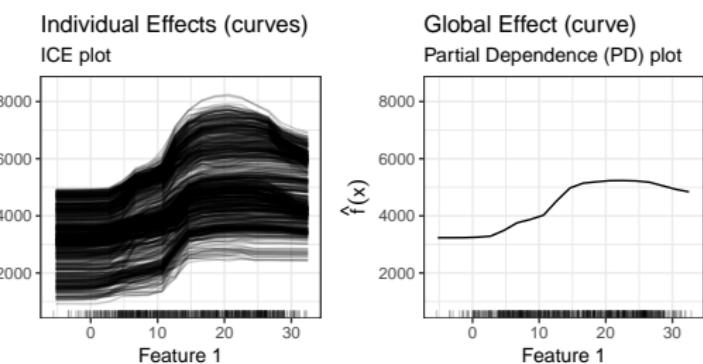


TYPES OF EXPLANATIONS

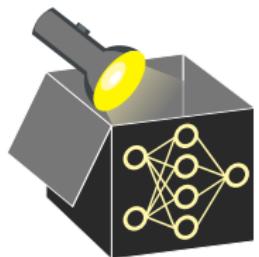
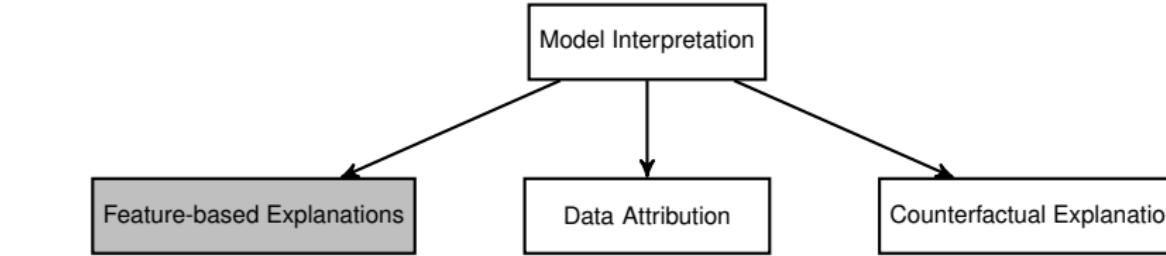


Feature Effects indicate changes (direction and magnitude) in model prediction due to changes in feature values.

- Model-agnostic methods:
ICE curves, PD plots ...
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Weights / coefficients θ_j
- Further examples: ALE,
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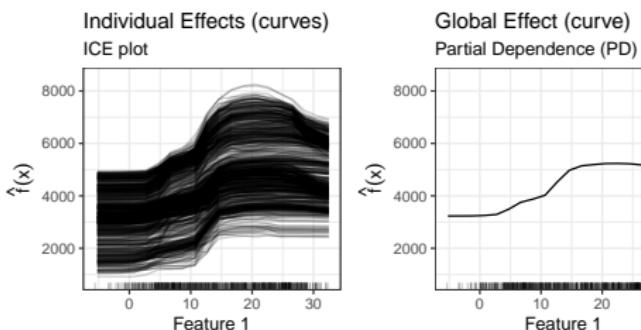


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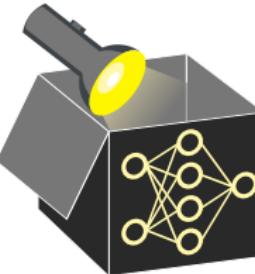
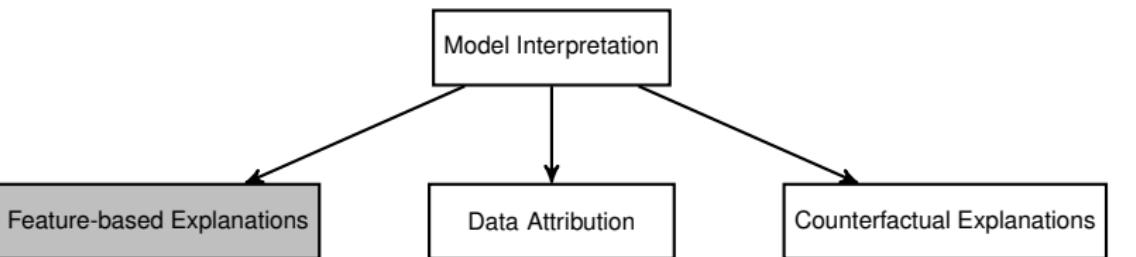


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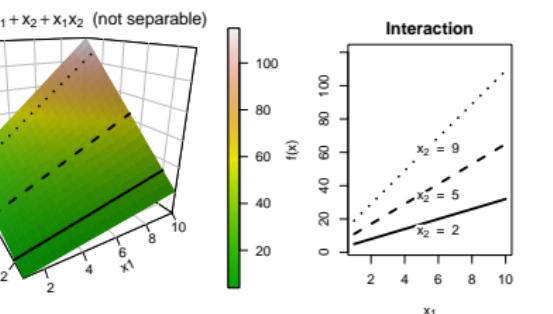


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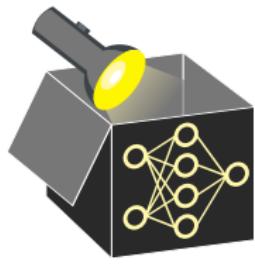
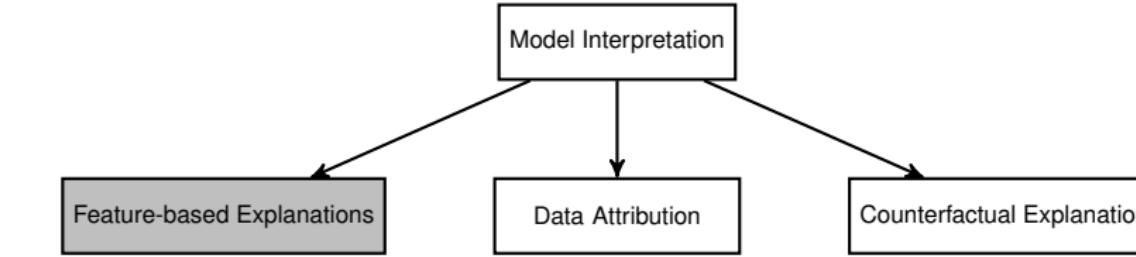


Feature Interaction: How combinations of features jointly affect predictions.

- Model-agnostic methods:
Friedman's H-statistic
- Pendant in linear models:
Coefficients of interaction terms θ_{jk}

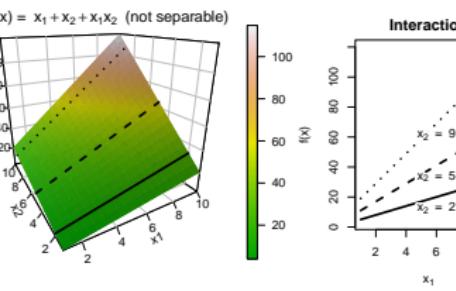


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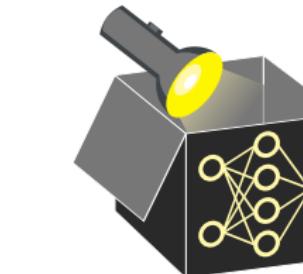
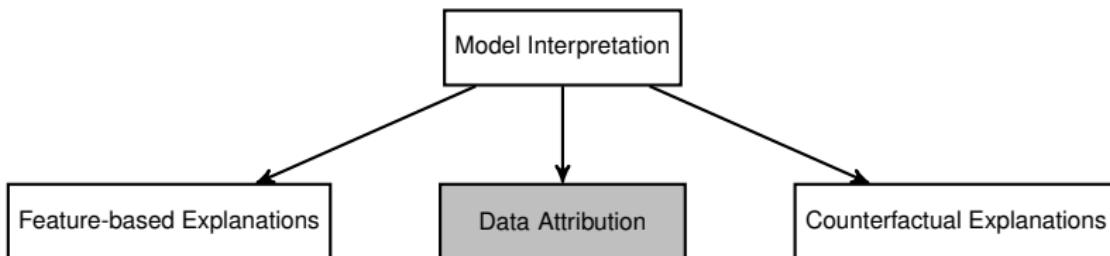


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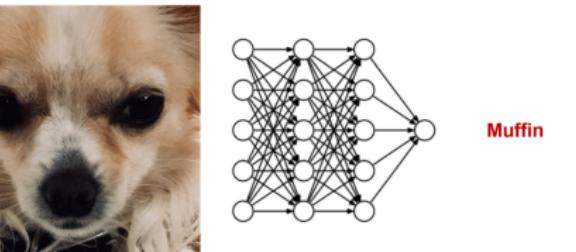
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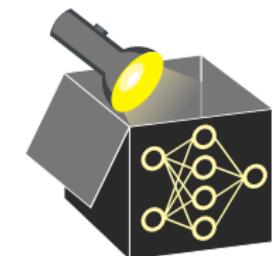
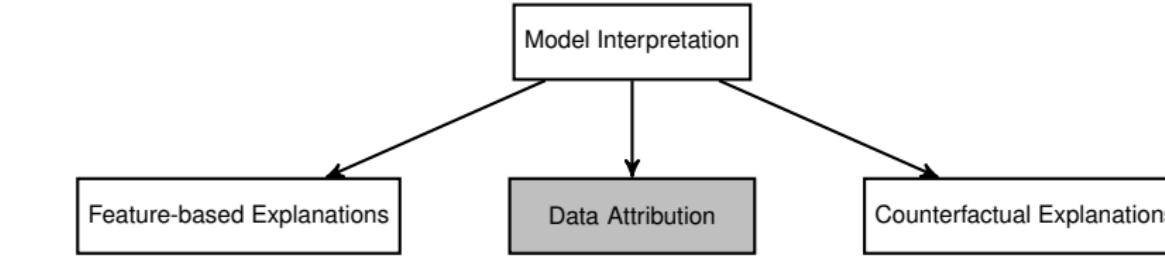
Data Attribution: Identify which training instances most influenced a prediction.

Example: A model should distinguish muffins and dogs.

Question: Why does it misclassify this dog image (test point) as a muffin?



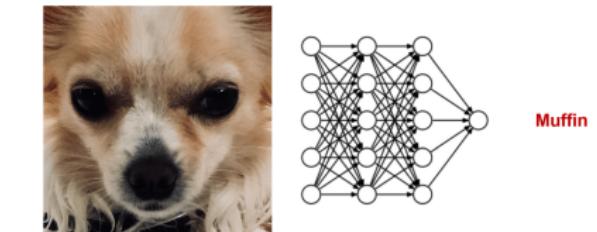
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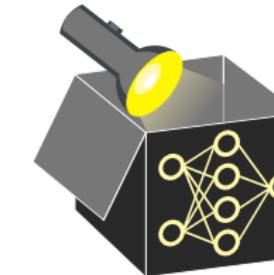
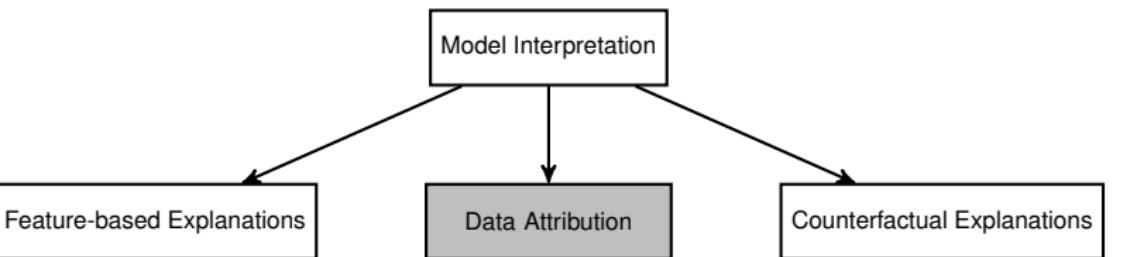
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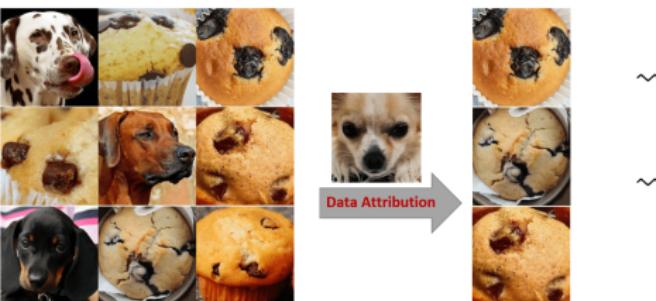
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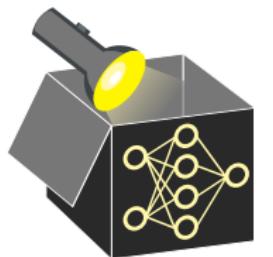
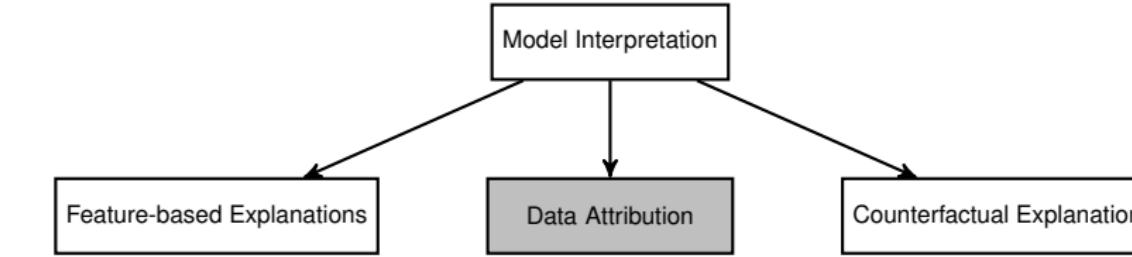
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Approach: Measure how perturbations to training instances affect prediction or loss.



- ~~ Influential training instances drive prediction of test points.
- ~~ If these resemble muffins, the model may predict muffin instead of dog.

TYPES OF EXPLANATIONS



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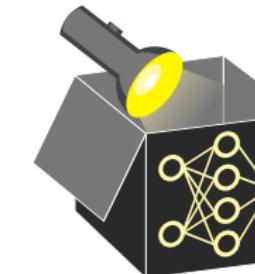
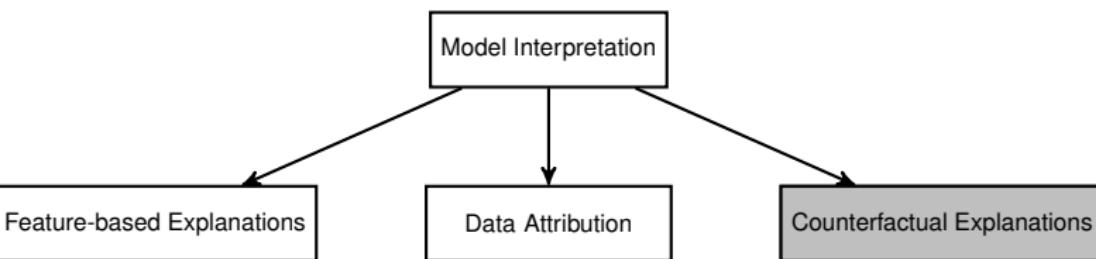
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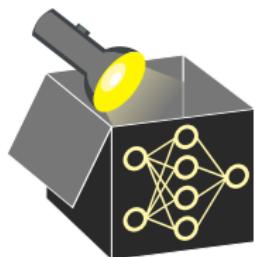
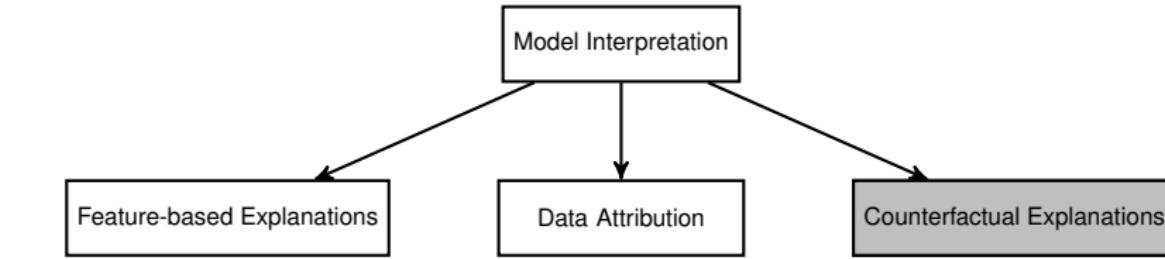


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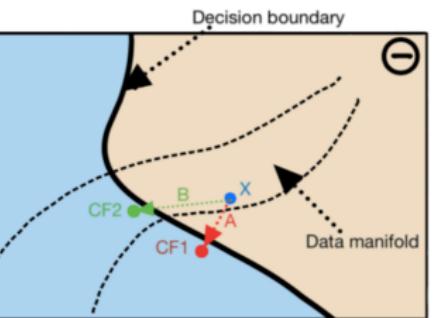


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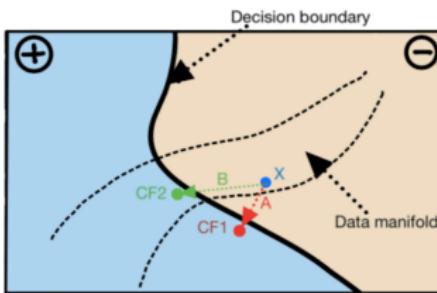
Counterfactual Explanations:

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

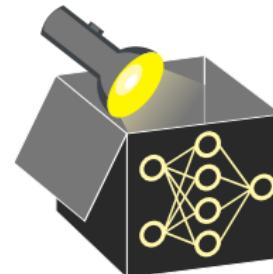
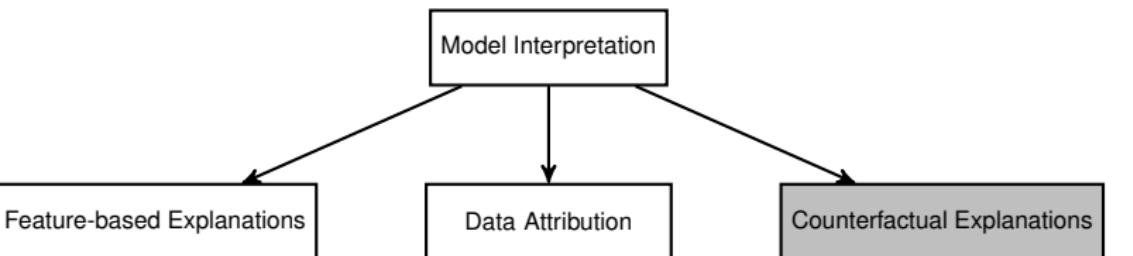


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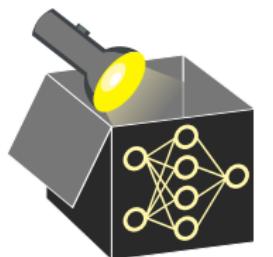
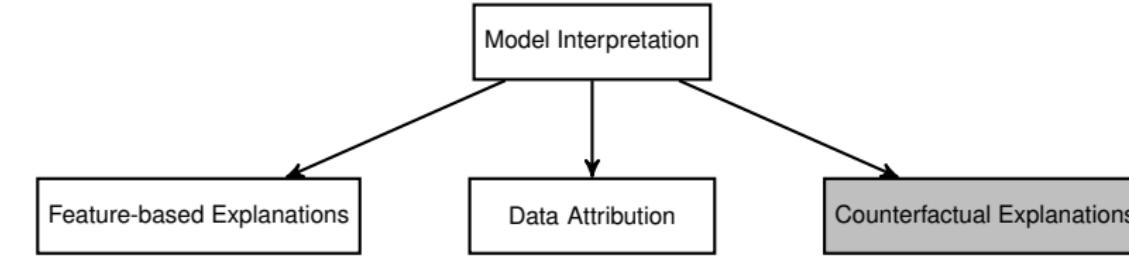
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What can a person do to obtain a favorable prediction from a given model ?



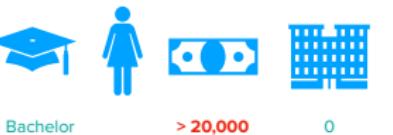
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LOCAL, GLOBAL, AND REGIONAL EXPLANATIONS

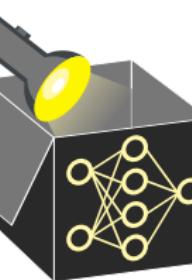
Local – Explain model behavior for **single instances**:

- Provide nuanced instance-specific insights
- Crucial for complex models where features typically affect instances differently (due to interactions)
- Examples: Counterfactuals, LIME, SHAP, ICE

Local



individual instance

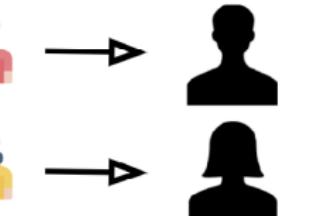


Global



"average" instance

Regional



"group" instance

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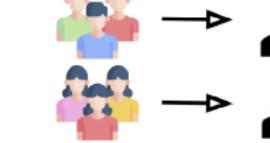
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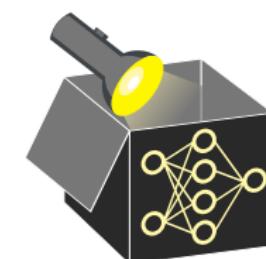


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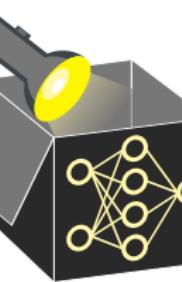
Global – Explain model behavior for **entire input space**:

- Provide high-level insights into model behavior, often by aggregating local explanations
- Easier to communicate but loss of detail & over-simplification (hides differences)
- Examples: PD plots, ALE plots, PFI

Local



individual instance

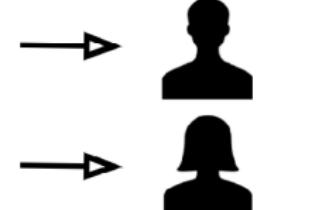


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Global: Explain model behavior for **entire input space**:

- Provide high-level insights into model behavior, often by aggregating local explanations
- Easier to communicate but loss of detail & over-simplification (hides differences)
- Examples: PD plots, ALE plots, PFI

Local



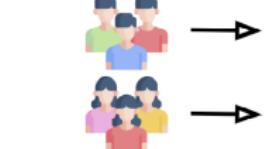
individual instance

Global

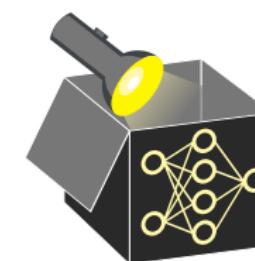


"average" instance

Regional



"group" instance



LOCAL, GLOBAL, AND REGIONAL EXPLANATIONS

Local – Explain model behavior for **single instances**:

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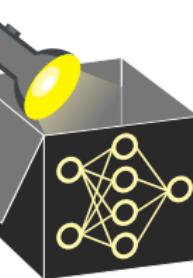
Regional explanations – for **subspaces / regions**:

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individual instance

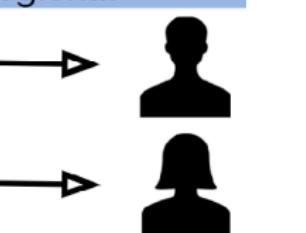


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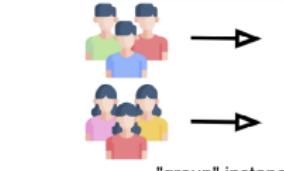
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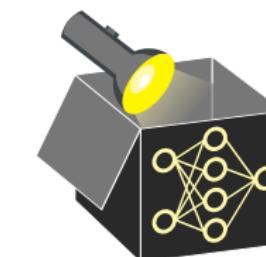


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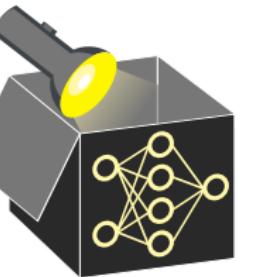
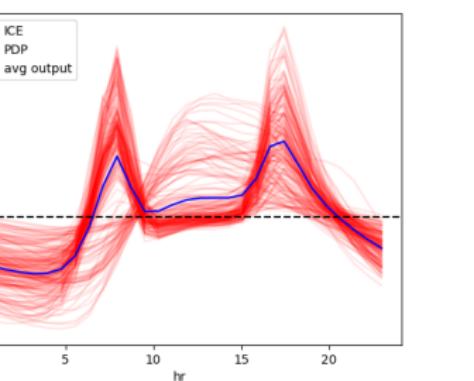


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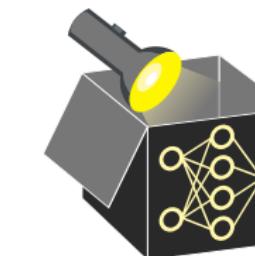
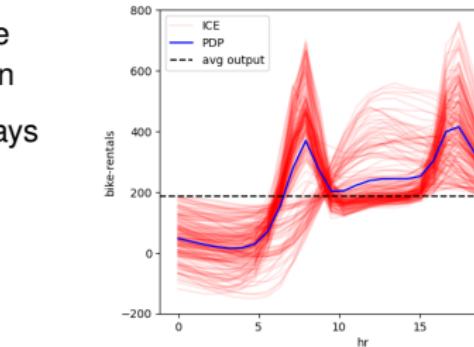
LOCAL, GLOBAL, AND REGIONAL EXPLANATIONS

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LOCAL, GLOBAL, REGIONAL EXPLANATIONS

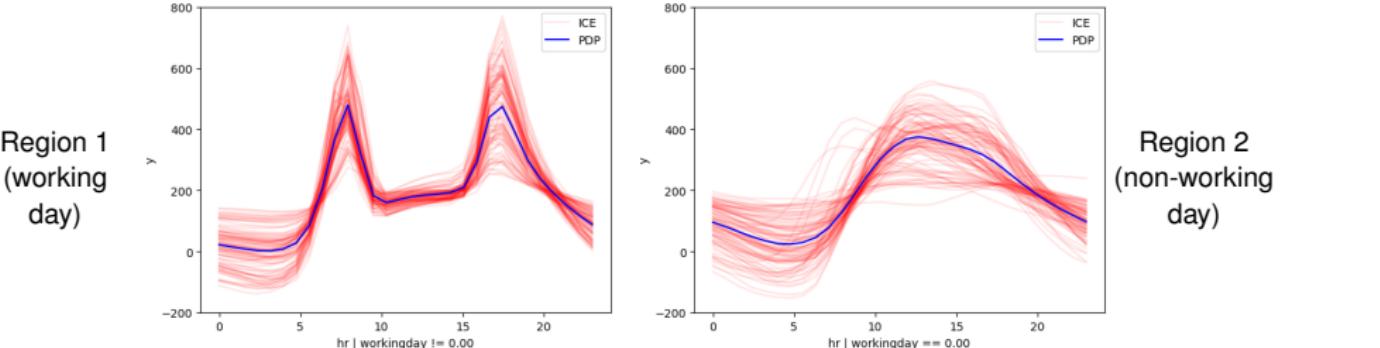
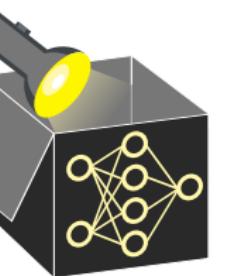
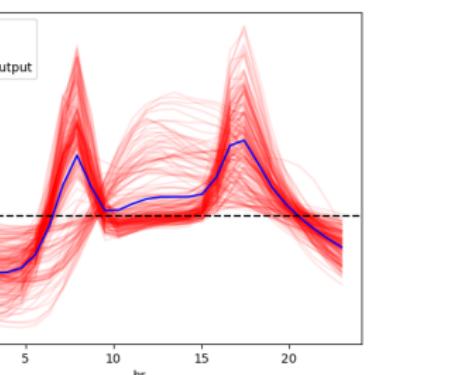
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 - Region 1: morning and evening peak
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~~ Preserves detail without overload (challenge: find regions automatically)

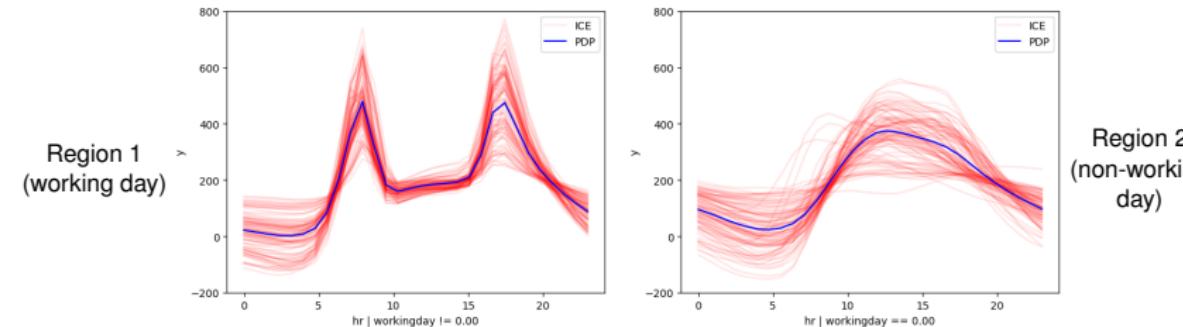
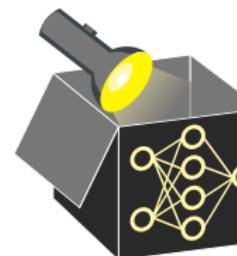
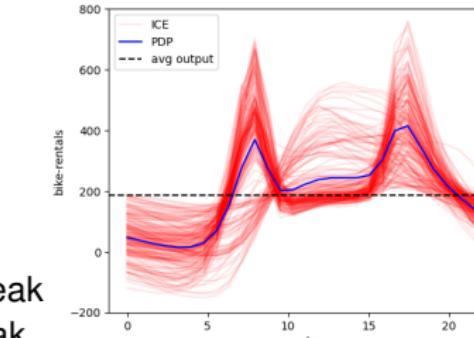


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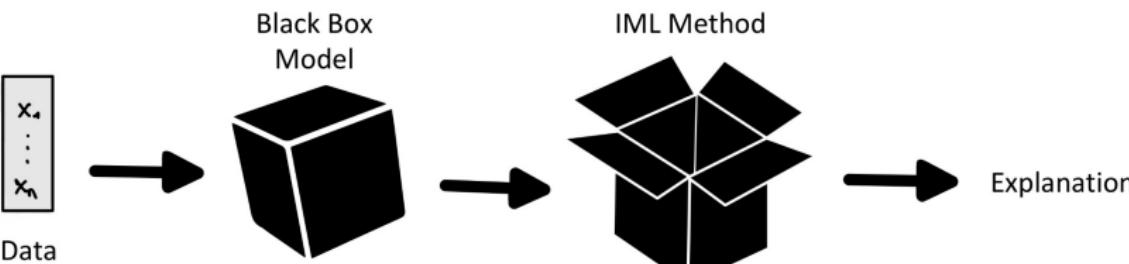
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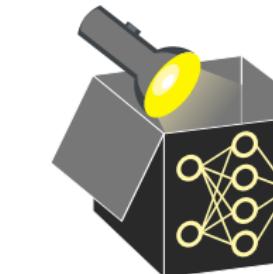


FIXED MODEL VS. REFITS

- Input of global interpretation methods: model + data, output: explanations
 - ~ Explanations can be viewed as statistical estimators

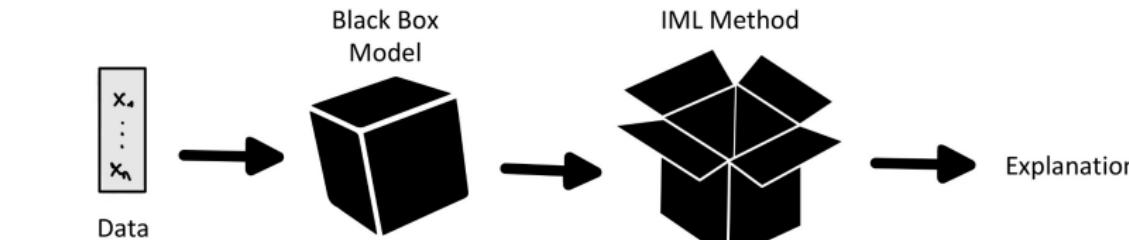


- Situation in ML: Deployed model is trained on all available data
 - ~ No unseen test data left to, e.g., reliably estimate performance
 - ~ IML method could use same data model was trained on
 - ~ But: Some IML methods rely on measuring loss requiring unseen test data
- Alternative: Explain the inducer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

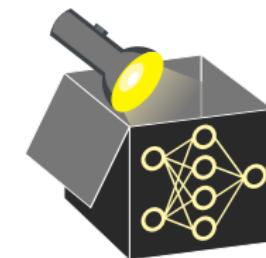


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LEVELS OF INTERPRETABILITY

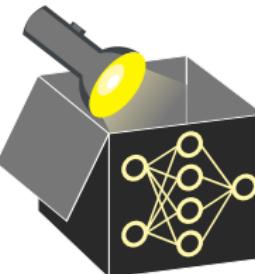
Research Question

1st
level
view

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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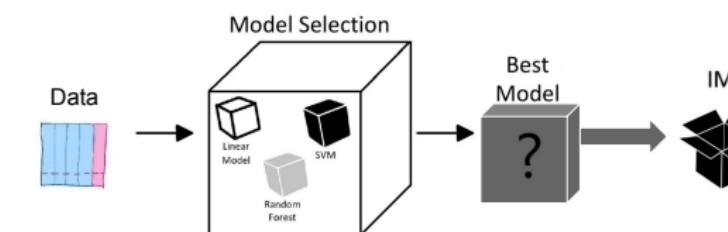
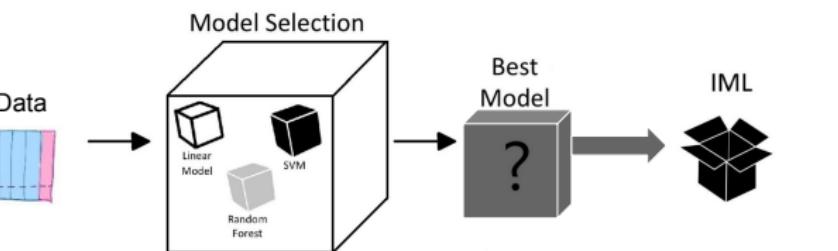
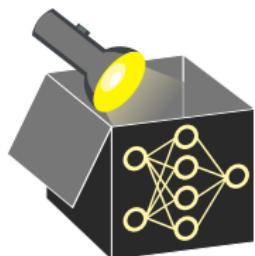
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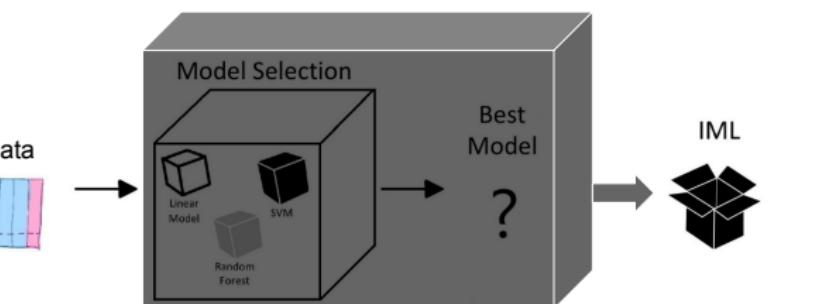
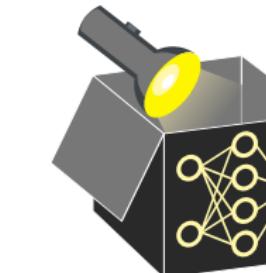
2nd
level
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Model selection process (e.g., decisions made by AutoML systems or HPO process)



LEVELS OF INTERPRETABILITY

Research Question

1st
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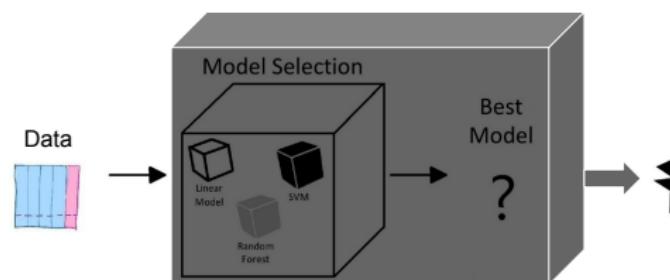
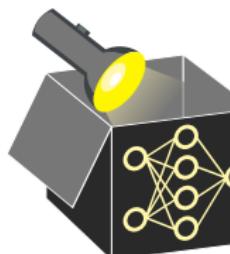
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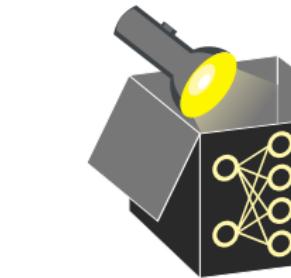
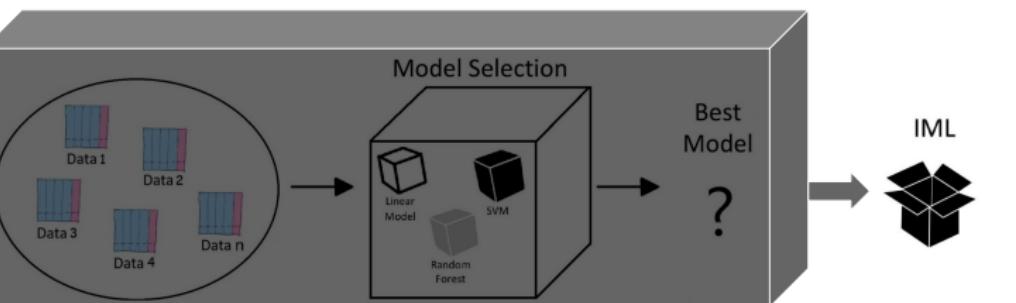
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LEVELS OF INTERPRETABILITY

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LEVELS OF INTERPRETABILITY

	Research Question	Objects of analysis
1 st level view	How to explain a given model fitted on a data set?	(deployed) model $\theta \mapsto \hat{f}(\theta)$
2 nd level view	How does an optimizer choose a model based on a data set?	Model selection process (e.g., decisions made by AutoML systems or HPO process)
3 rd level view	How do data properties relate to performance of a learner and its hyperparameters?	Properties of ML algorithms in general (benchmark)

