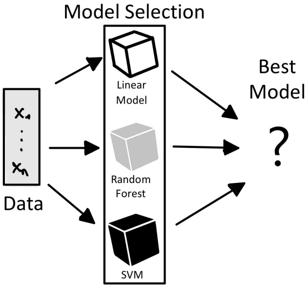
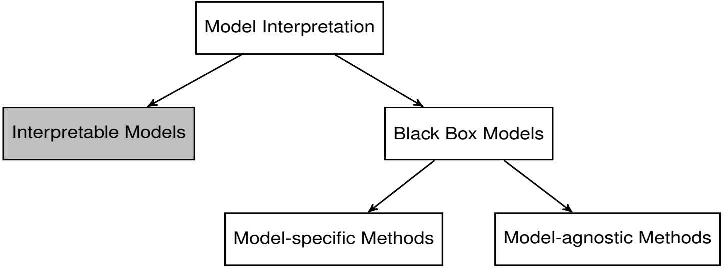
Interpretable Machine Learning
Dimensions of Interpretability

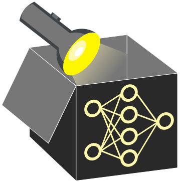


Learning goals

- Difference between intrinsic, model-specific, and model-agnostic interpretability
- Different types of explanations
- Local, global, and regional explanations
- Model/learner explanation (with(out) refits)
- Levels of interpretability

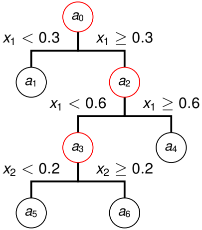
INTRINSIC, MODEL-SPECIFIC, MODEL-AGNOSTIC





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 (many features/interactions)



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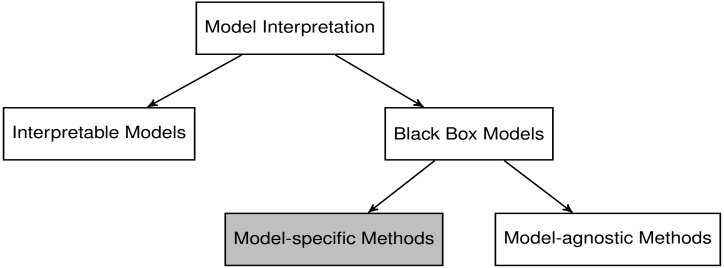
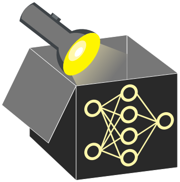
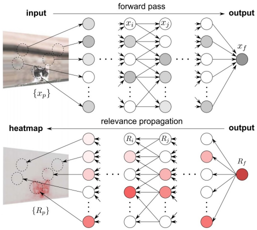




Model-specific Methods:

- Designed for specific model types (e.g., NNs)
- Examples:
  Gini importance of tree-based models,
  Layer-wise relevance propagation (LRP)
- Pro: Exploit model structure
- Con: Restricted to specific model class



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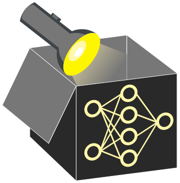
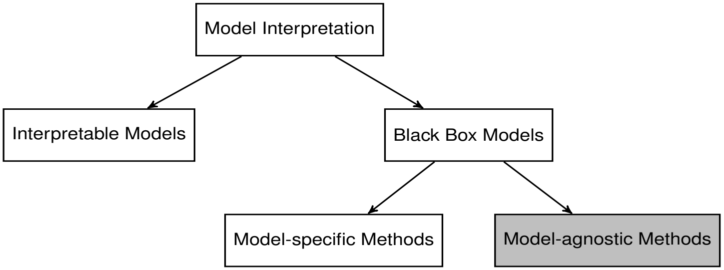
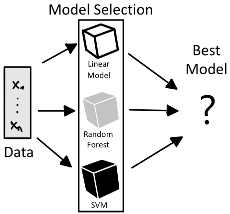


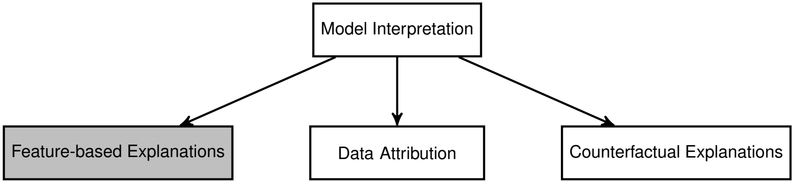


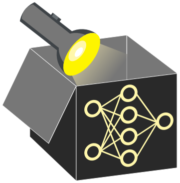
Model-agnostic Methods:

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



TYPES OF EXPLANATIONS

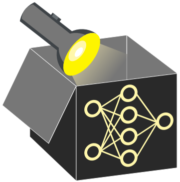


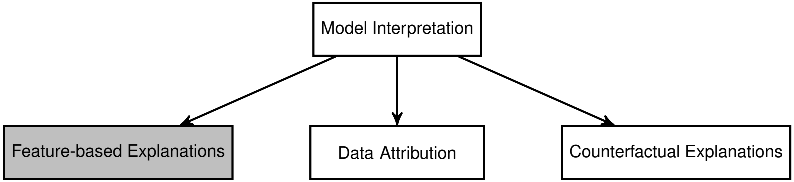


Feature-based Explanations:

- 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.

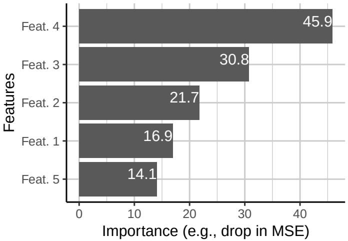
TYPES OF EXPLANATIONS





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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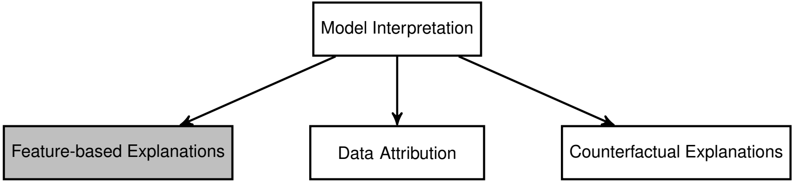
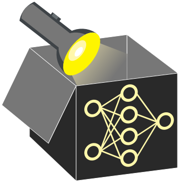
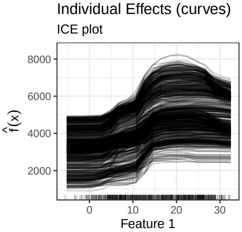
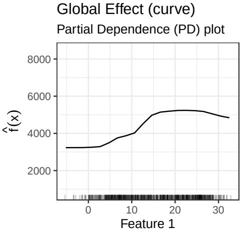




Feature Effects indicate changes (direction and magnitude) in model prediction due to changes in feature values.

- Model-agnostic methods: ICE curves, PD plots . . .
- Pendant in linear models: Weights / coefficients θ_j
- Further examples: ALE, SHAP, and LIME





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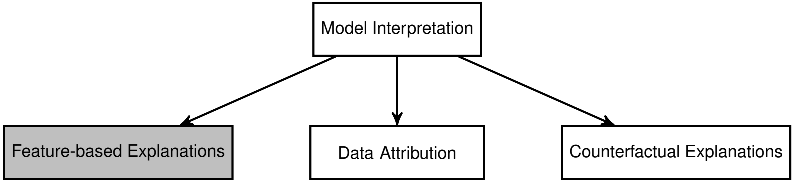
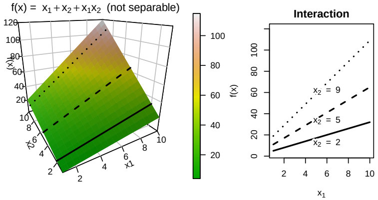


Feature Interaction:
How combinations of features jointly affect predictions.

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



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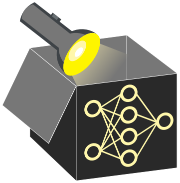


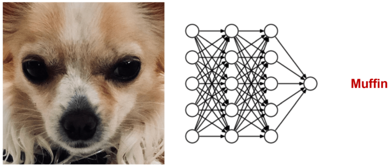
Model Interpretation

Feature-based Explanations | Data Attribution | Counterfactual Explanations

Data Attribution: Identify training instances that 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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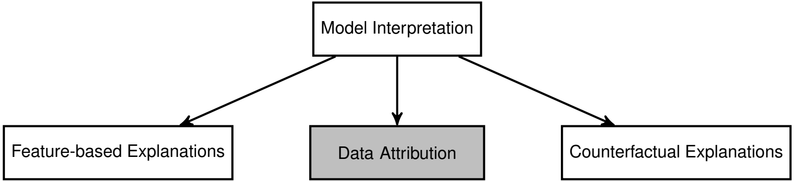
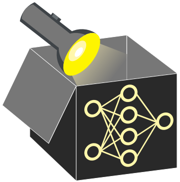




Data Attribution: Identify training instances that most influenced a prediction.

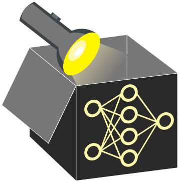
Example: A model should distinguish muffins and dogs.

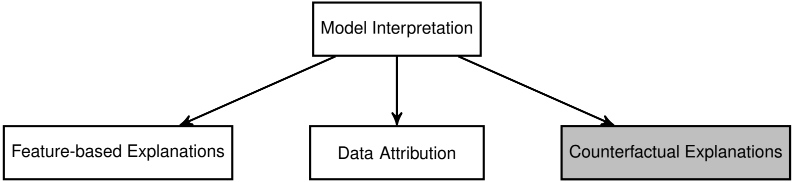
Approach: Measure how perturbations to training data affect prediction/loss.

⇝ Influential training instances drive prediction of test points.

⇝ If these resemble muffins, the model may predict muffin instead of dog.

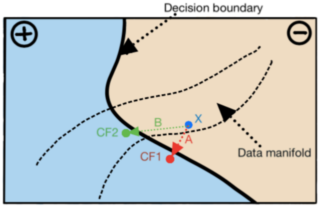
TYPES OF EXPLANATIONS





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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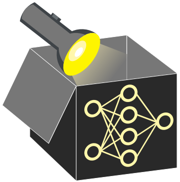
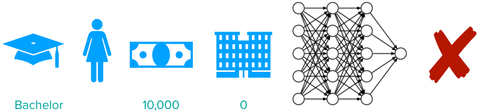


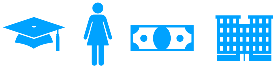
Model Interpretation

- Feature-based Explanations
- Data Attribution
- Counterfactual Explanations

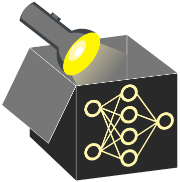
Example (loan application):



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

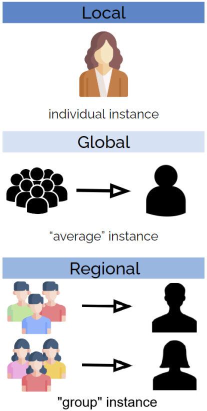


LOCAL, GLOBAL, AND REGIONAL EXPLANATIONS



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



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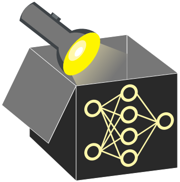

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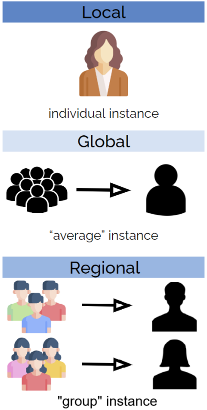
Global: Explain model behavior for **entire input space**:

- 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



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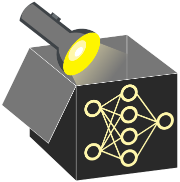

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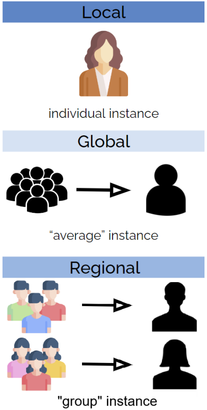
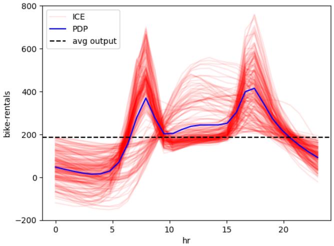
Regional explanations – for **subspaces** / **regions**:

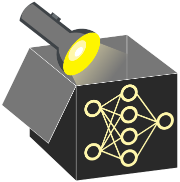
- Compromise between nuanced & high-level insights
- Useful when local explanations group well without losing much detail



LOCAL, GLOBAL, REGIONAL EXPLANATIONS

- **Local** (red): ICE curves for one instance
  $\rightsquigarrow$ Detailed but cluttered/obscure pattern
- **Global** (blue): PDP averaged over *all* days
  $\rightsquigarrow$ Averaged curve hides heterogeneity





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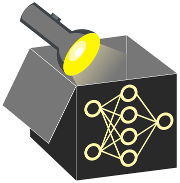

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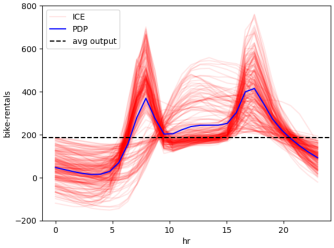
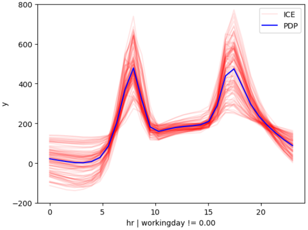
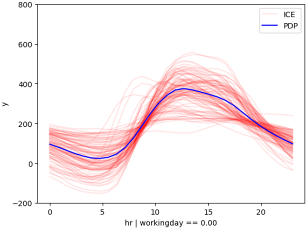
- **Regional**: Split data on `workingday`
  - Region 1: morning and evening peak
  - Region 2: late-morning leisure peak

  $\rightsquigarrow$ Preserves detail without overload
  $\rightsquigarrow$ Challenge: find regions automatically



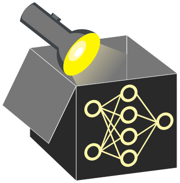
Region 1 (working day)



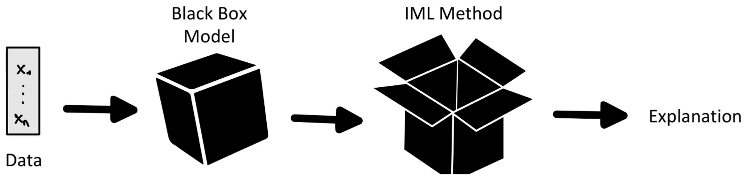


Region 2 (non-working day)

FIXED MODEL VS. REFITS

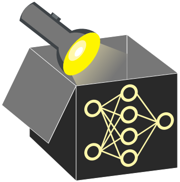


- Global interpretation methods: Input: model + data, output: explanations
  $\rightsquigarrow$ Explanations can be viewed as statistical estimators

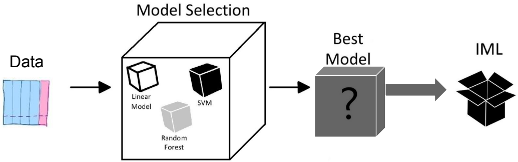


- Situation in ML: Deployed model is trained on all available data
  $\rightsquigarrow$ No unseen test data left to, e.g., reliably estimate performance
  $\rightsquigarrow$ IML method could use same data model was trained on
  $\rightsquigarrow$ But: Some IML methods require measuring loss on unseen test data
- Alternative: Explain the inducer that created the model (not a fixed model)
  $\rightsquigarrow$ Idea: Use resample strategies (e.g. CV) as in performance estimation
  $\rightsquigarrow$ Requires refitting

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



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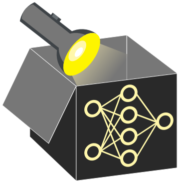

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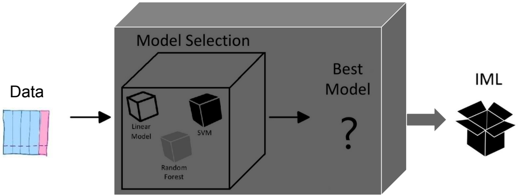

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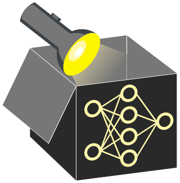

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3^{rd} level view	How do data properties relate to performance of a learner and its hyperparameters?	Properties of ML algorithms in general (benchmark)