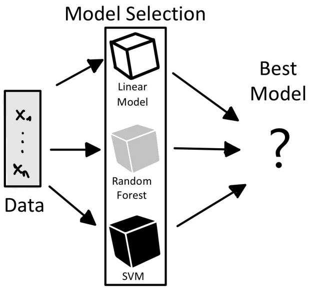
Interpretable Machine Learning

Intro to IML

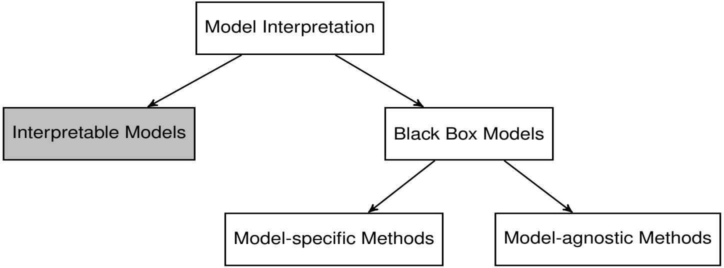
Dimensions of Interpretability

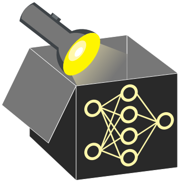


Learning goals

- 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

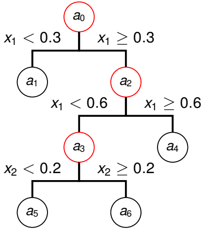
INTRINSIC, MODEL-SPECIFIC, MODEL-AGNOSTIC





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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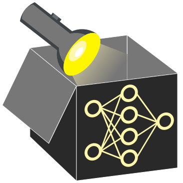
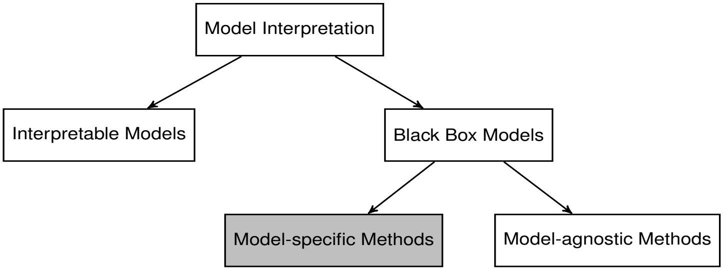
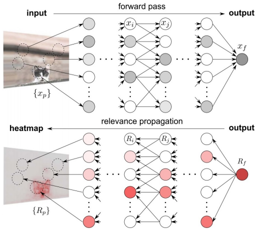




Model-specific Methods:

- 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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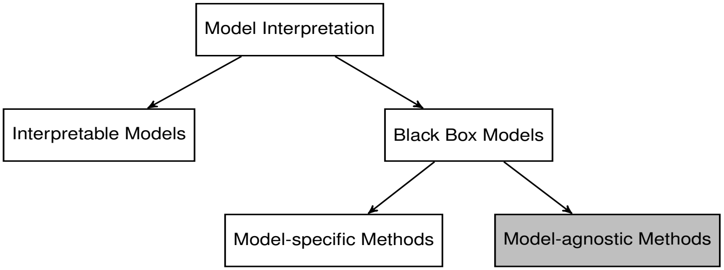
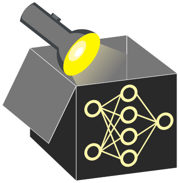
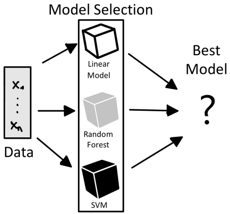


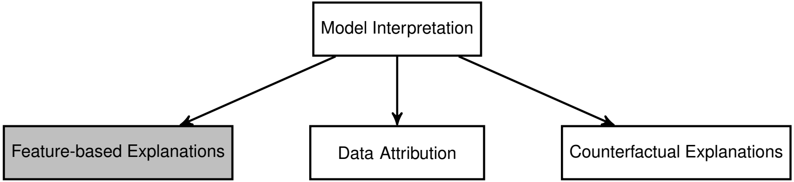


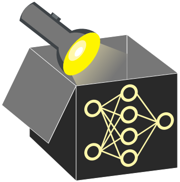
Model-agnostic Methods:

- 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.

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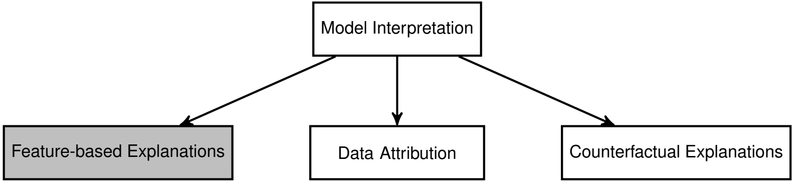
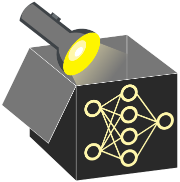
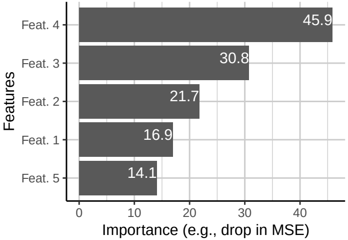




Feature Importance quantifies relevance of features, e.g., their contribution to model prediction, predictive performance, or prediction variance.

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



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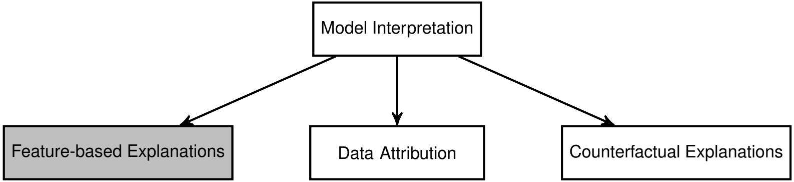
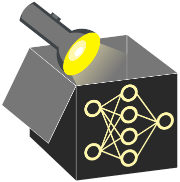
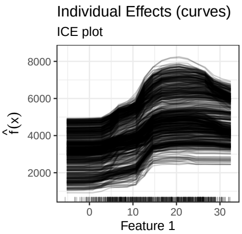
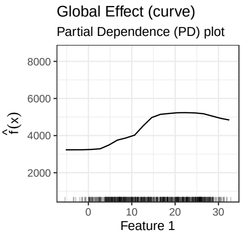




Feature Effects indicate changes (direction and magnitude) in model prediction due to changes in feature values.

- 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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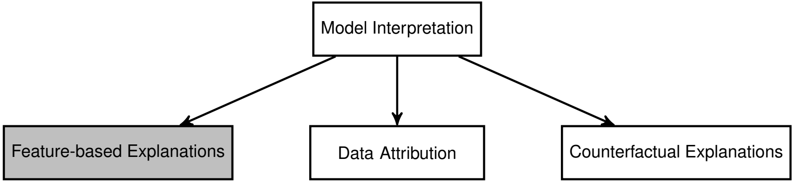
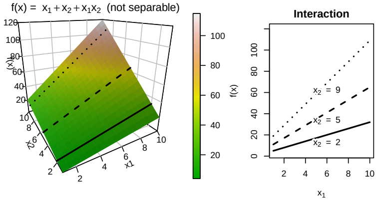


Feature Interaction:
How combinations of features jointly affect predictions.

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



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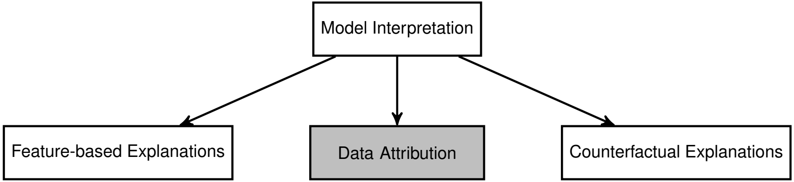
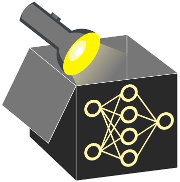
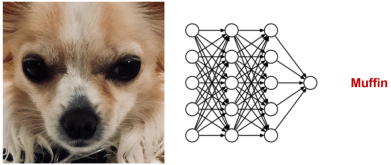




Data Attribution: Identify training instances that most influenced a prediction.

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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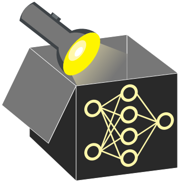

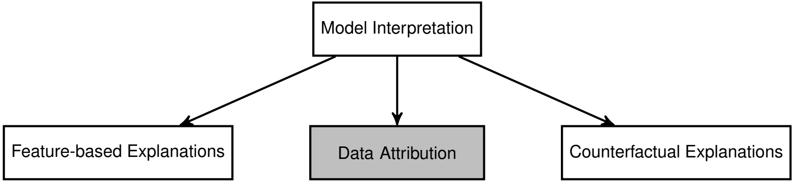

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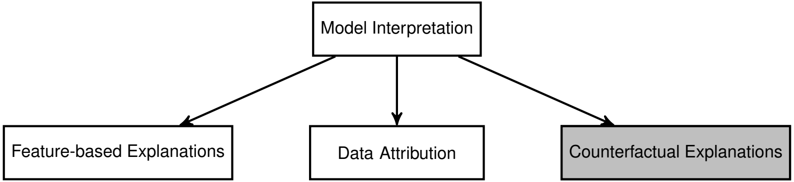
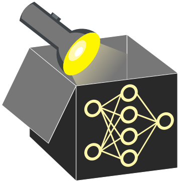
Approach: Measure how perturbations to training data affect prediction/loss.

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

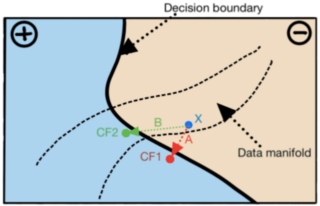
TYPES OF EXPLANATIONS





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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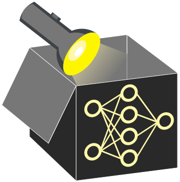
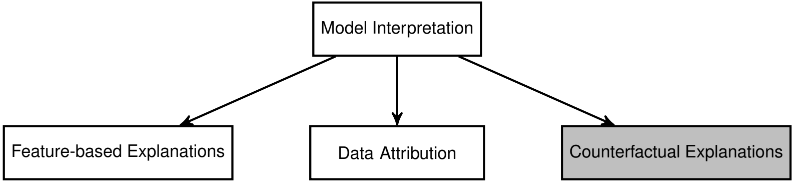
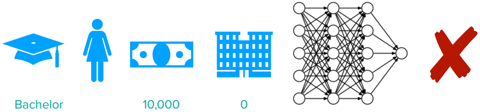
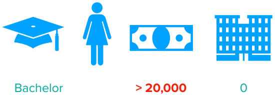




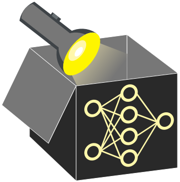
Example (loan application):



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

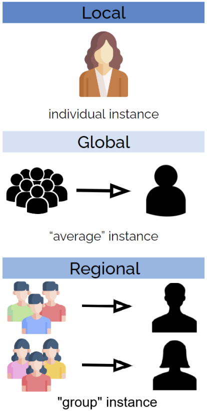


LOCAL, GLOBAL, AND REGIONAL EXPLANATIONS



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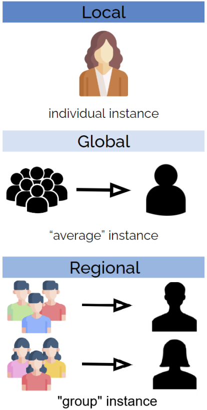
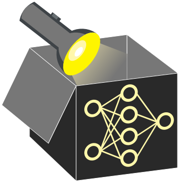
Global: Explain model behavior for **entire input space**:

- 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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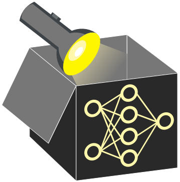

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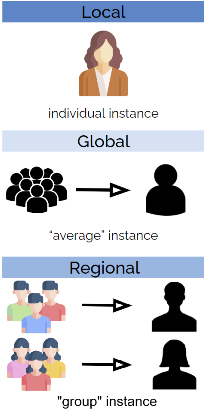
Regional explanations – for **subspaces** / **regions**:

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



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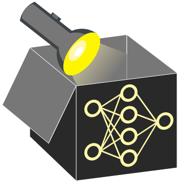
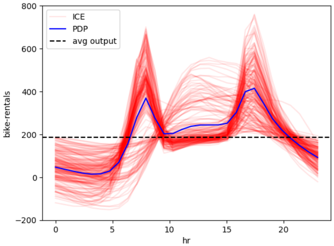


- **Local** (red): ICE curves for one instance
  $\rightsquigarrow$ Detailed but cluttered/obscure pattern
- **Global** (blue): PDP averaged over *all* days
  $\rightsquigarrow$ Averaged curve hides heterogeneity



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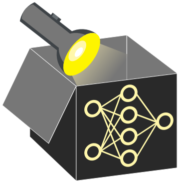

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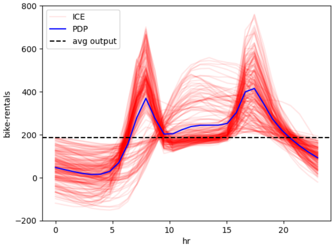
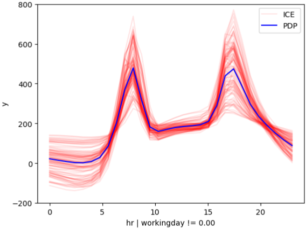
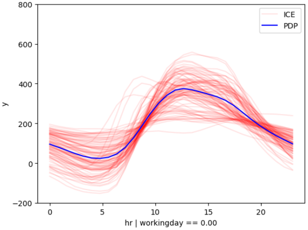
  $\rightsquigarrow$ Averaged curve hides heterogeneity
- **Regional**: Split data on `workingday`
  - Region 1: morning and evening peak
  - Region 2: late-morning leisure peak

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



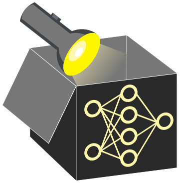
Region 1
(working day)



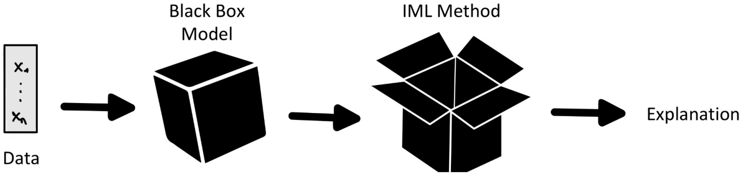


Region 2
(non-working
day)

FIXED MODEL VS. REFITS

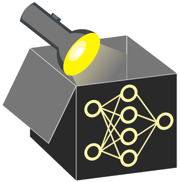


- Global interpretation methods: Input: model + data, output: explanations
  $\rightsquigarrow$ Explanations can be viewed as statistical estimators

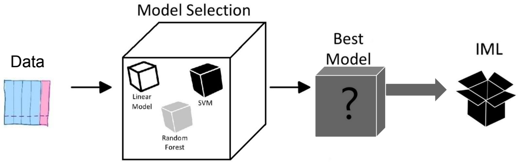


- Situation in ML: Deployed model is trained on all available data
  $\rightsquigarrow$ No unseen test data left to, e.g., reliably estimate performance
  $\rightsquigarrow$ IML method could use same data model was trained on
  $\rightsquigarrow$ But: Some IML methods require measuring loss on unseen 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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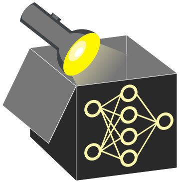

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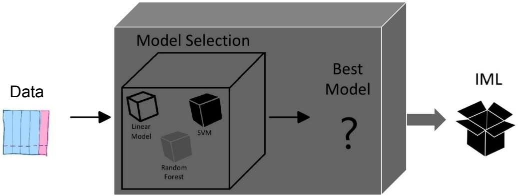

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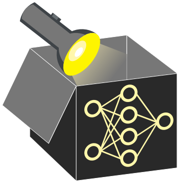

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2^{nd} level view	How does an optimizer choose a model based on a data set?	Model selection process (e.g., decisions made by AutoML systems or HPO)
3^{rd} level view	How do data properties relate to performance of a learner and its hyperparameters?	Properties of ML algorithms in general (benchmark)