Interpretable Machine Learning

Introduction to loss-based feature importance

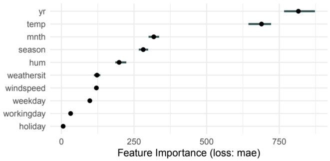
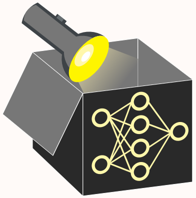


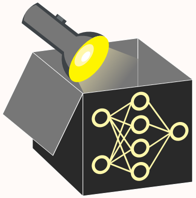
Figure: Bike Sharing Dataset



Learning goals

- Understand motivation for feature importance
- Develop an intuition for possible use-cases
- Know characteristics of feature importance methods

MOTIVATION



- **Feature effects** describe the relationship of features x with the prediction $\hat{y}$
  - requires one plot per feature
  - does not take the true target y into account

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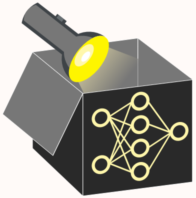

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- **Feature importance** methods quantify the relevance of features w.r.t. prediction performance
  - condensed to one number per feature
  - provides insight into the relationship with y

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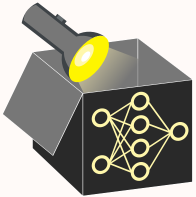

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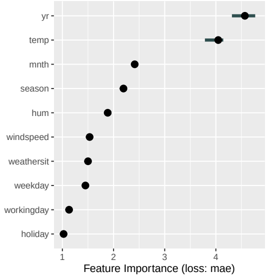
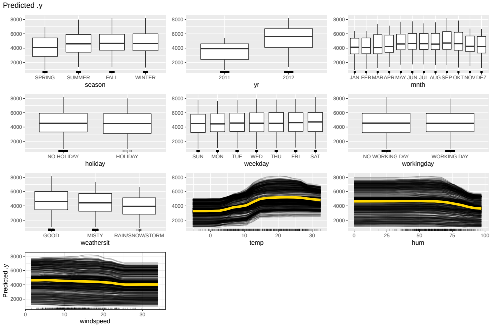
  - provides insight into the relationship with y
- **N.B.**: Here, we use the term feature importance to describe loss-based feature importance methods. In the literature, you may find other notions of "feature importance" (e.g., variance-based methods derived from feature effect methods, see also ▸ Greenwell et al. (2020))

EXAMPLE

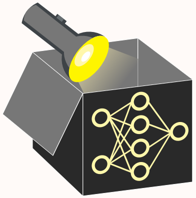
Feature importance offers a condensed summary of the relevance of features w.r.t. performance

- Fit random forest on bike sharing data
- Left: Feature importance ranking by permutation feature importance (PFI)
- Right: Feature effects for all features





FEATURE IMPORTANCE SCHEME

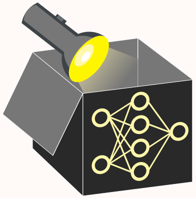


Loss-based feature importance methods are often based on two concepts

1. **Perturbation/Removal:**
   Generate predictions for which the feature of interest has been perturbed or removed
2. **Performance Comparison:**
   Compare performance under perturbation/removal with the original model performance

Depending on the type of perturbation/removal, feature importance methods provide insight into different aspects of model and data.

POTENTIAL INTERPRETATION GOALS



Feature importance methods provide condensed insights, but can only highlight certain aspects of model and data. There are different interpretation goals one might be interested in whose question of interest do not necessarily coincide (except for special cases).

For example, one may be interested in getting insight into whether the ...

(1) feature x_j is causal for the prediction?

(2) feature x_j contains prediction-relevant information about y?

(3) model requires access to x_j to achieve it's prediction performance?

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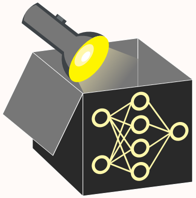

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For example, one may be interested in getting insight into whether the ...

(1) feature x_j is causal for the prediction?

- Changing feature value x_j has an effect on prediction $\hat{y} = \hat{f}(x)$
- In LM: non-zero coefficient, in ML: present feature effect
- **Note:** If x_j is causal for prediction $\hat{y} \not\Rightarrow$ causal for the ground truth y, e.g.:
  - A disease symptom may be used in a model to predict disease status $\leadsto$ causal for prediction $\hat{y}$
  - But intervening on disease symptom does not have an effect on the disease $\leadsto$ not causal for the ground truth y

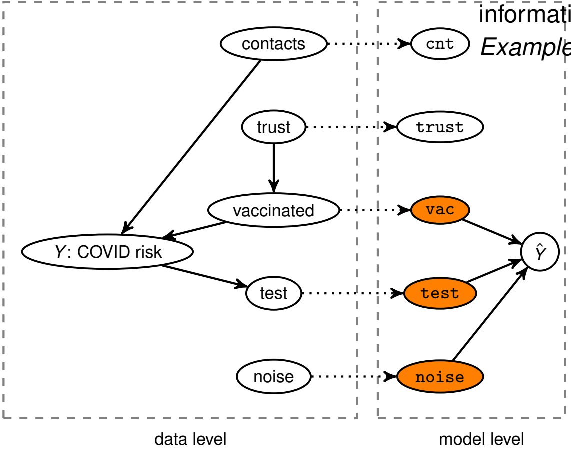
(2) feature x_j contains prediction-relevant information about y?

(3) model requires access to x_j to achieve it's prediction performance?

EXAMPLE: CAUSAL FOR THE PREDICTION (1)

A feature may be causal for the prediction $\hat{y}$ (1) without containing prediction-relevant information about y (2)

Examples: overfitting due noisy features



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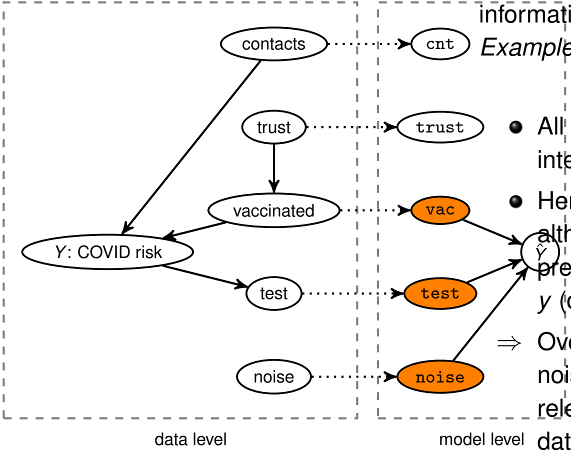
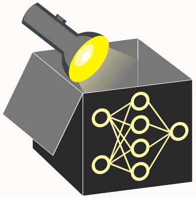


A feature may be causal for the prediction $\hat{y}$ (1) without containing prediction-relevant information about y (2)
Examples: overfitting due noisy features

- All features used by the model are of interest
- Here: Model uses feature `noise`, although it does not contain prediction-relevant information about y (data level)

$\Rightarrow$ Overfitted models may use many noise features which are deemed relevant on model level (but not on data level)



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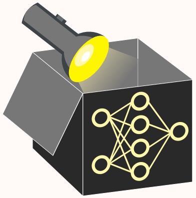


Feature importance methods provide condensed insights, but can only highlight certain aspects of model and data. There are different interpretation goals one might be interested in whose question of interest do not necessarily coincide (except for special cases).

For example, one may be interested in getting insight into whether the ...

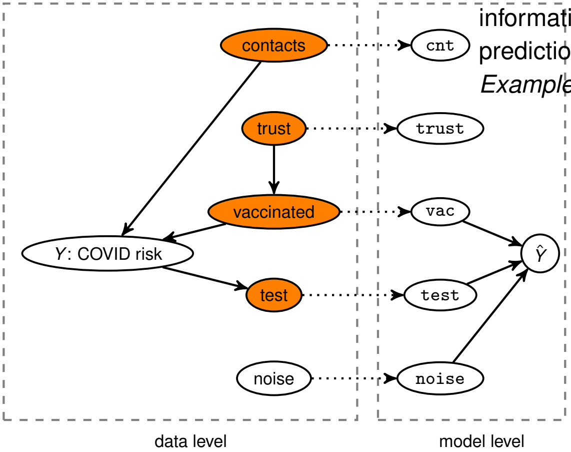
(1) feature x_j is causal for the prediction?

(2) feature x_j contains prediction-relevant information about y?

- Feature x_j helps to predict the target y (e.g., conditional expectation) w.r.t. performance
- If $x_j \perp y$ (independent) then x_j and y have zero mutual information (since $\mathbb{E}[y|x_j] = \mathbb{E}[y]$)
  $\leadsto$ x_j has no prediction-relevant information

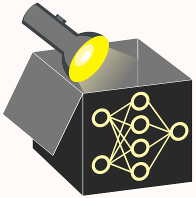
(3) model requires access to x_j to achieve it's prediction performance?

EXAMPLE: CONTAINS PREDICTION-RELEVANT INFORMATION (2)



A feature may contain prediction-relevant information (2) without causing the prediction (1)

Examples: underfitting, model multiplicity



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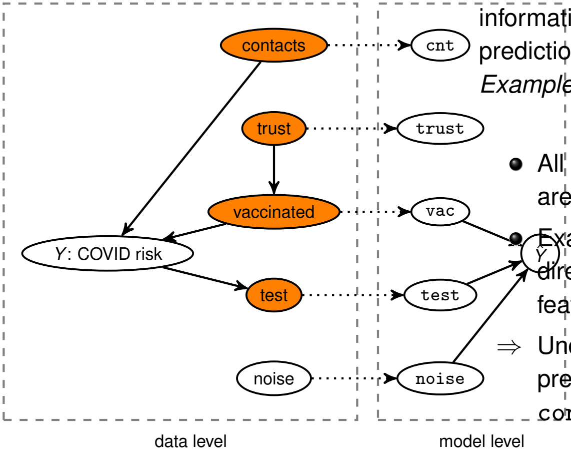


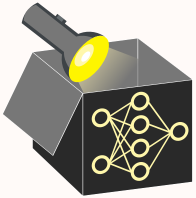
A feature may contain prediction-relevant information (2) without causing the prediction (1)

Examples: underfitting, model multiplicity

- All prediction-relevant features for y are of interest
- Example: All features that are directly or indirectly (i.e., via another feature) connected to y

$\Rightarrow$ Underfitted models may ignore prediction-relevant features such as `contacts` here

POTENTIAL INTERPRETATION GOALS



Feature importance methods provide condensed insights, but can only highlight certain aspects of model and data. There are different interpretation goals one might be interested in whose question of interest do not necessarily coincide (except for special cases).

For example, one may be interested in getting insight into whether the ...

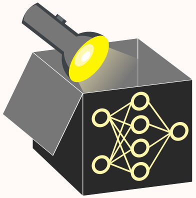
(1) feature x_j is causal for the prediction?

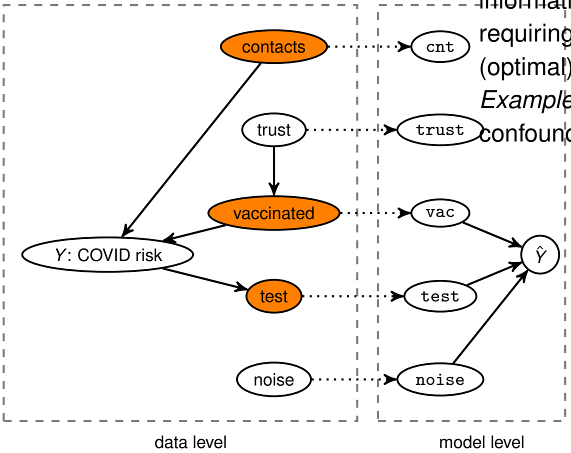
(2) feature x_j contains prediction-relevant information about y?

(3) model requires access to x_j to achieve it's prediction performance?

- Feature x_j helps to predict the target y w.r.t. performance, compared to using only x_{-j}
- If $x_j \perp y | x_{-j}$ (independent) then $\mathbb{E}[y|x_{-j}] = \mathbb{E}[y|x_j, x_{-j}]$
  $\rightsquigarrow$ x_j does not contribute unique prediction-relevant information about y
- **Note:** A model may rely on features that can be replaced with others, e.g., a random forest fitted on data with $\mathbb{E}[y|x_1] \neq \mathbb{E}[y]$ and $\mathbb{E}[y|x_1] = \mathbb{E}[y|x_1, x_2]$ where x_1 was not used as split variable may rely on x_2

EXAMPLE: UNIQUE PREDICTION RELEVANT INFORMATION (3)





A feature may contain prediction-relevant information (2), without the model requiring access to the feature for (optimal) prediction performance (3)

Examples: correlated features, confounding

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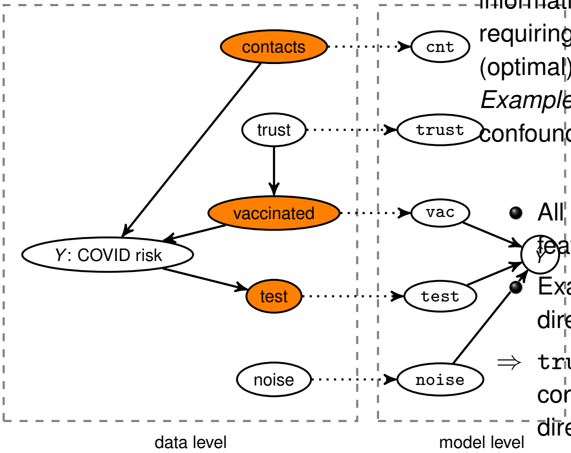

A feature may contain prediction-relevant information (2), without the model requiring access to the feature for (optimal) prediction performance (3)
Examples: correlated features, confounding

- All unique prediction-relevant features for y are of interest
- Example: All features that are directly connected to y

$\Rightarrow$ `trust` and `vaccinated` may be correlated but only `vaccinated` is directly connected to y