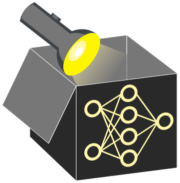
Interpretable Machine Learning

Feature Importance

Intro to Loss-based Feature Importance



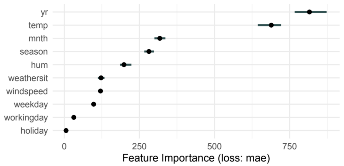
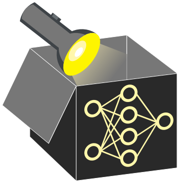


Figure: Bike Sharing Dataset

Learning goals

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

MOTIVATION



- **Feature effects** describe how a feature x_j influences the prediction $\hat{y}$
  - requires one plot per feature (e.g., PDPs, ALEs)
  - purely model-based; ignores true target y

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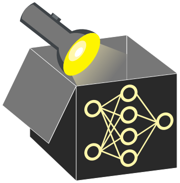

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  - condenses information into one number per feature
  - typically compares prediction errors (involves y) with/without feature

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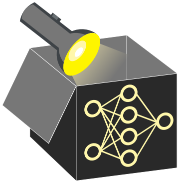

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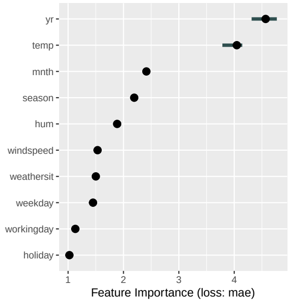
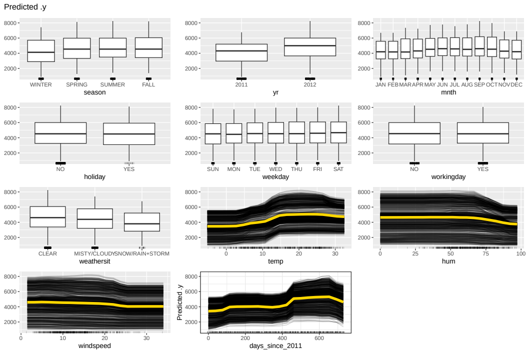
  - condenses information into one number per feature
  - typically compares prediction errors (involves y) with/without feature
- **Clarification:** By *feature importance*, we mean *loss-based* methods that assess a feature's impact via changes in *prediction error*.
  $\rightsquigarrow$ Other notions exist (e.g., variance-based methods; see ▸ "Greenwell et al." 2020).

EXAMPLE

Feature importance provides a condensed summary of feature relevance w.r.t. performance

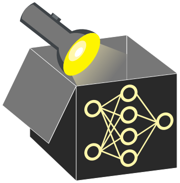
- Fit random forest on bike sharing data
- Left: Feature importance ranking by permutation feature importance (PFI)
- Right: Feature effects for all features





FEATURE IMPORTANCE - DIFFERENCES

▸ "Ewald et al." 2024



Many loss-based feature importance methods exist, which mainly differ in

(1) How they "remove" or "perturb" the feature of interest (FOI) X_j

- **Remove** X_j **and refit:** Drop the X_j and retrain model without it
- **Perturb** X_j**:** Replace X_j by $\tilde{X}_j$ sampled from *marginal*/*conditional* distrib.
- **Marginalize** X_j**:** integrate out X_j via *marginal* or *conditional* distribution

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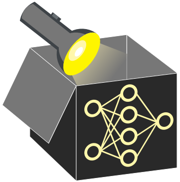

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(2) How they compare model performance before and after feat. removal

- **Compare "reduced model" without FOI vs. full model**:
  Measure drop in performance when FOI is "removed"
  $\rightsquigarrow$ Similar idea as backward feature elimination
- **Compare "empty model" (no features) vs. model with only FOI**:
  Measure gain in performance when only FOI is used
  $\rightsquigarrow$ Similar idea as forward feature selection
- **Compare models with/without FOI across different feature sets**:
  Measure average contrib. when FOI joins any feat. set (Shapley-based)

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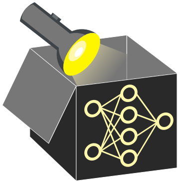

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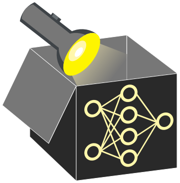
Depending on the different removal/perturbation and comparison strategies, feat. imp. methods provide insight into different aspects of model and data.

POTENTIAL INTERPRETATION GOALS



Feature importance methods provide condensed insights, but only into specific aspects of model and data. Interpretation goals often differ and typically address non-overlapping questions (except for special cases).

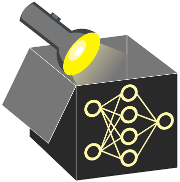
For example, one may be interested in getting insight into whether the ...

(1) feature x_j is causal for the prediction?

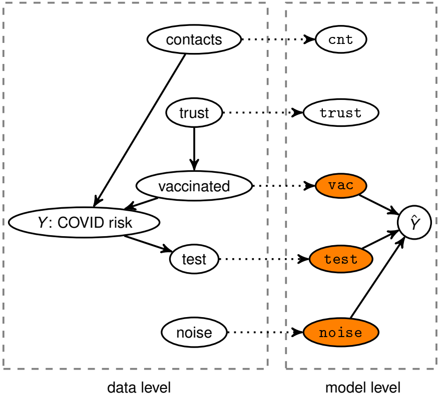
(2) feature x_j contains prediction-relevant information about y?

(3) model requires access to x_j to achieve its prediction performance?

EXAMPLE: CAUSAL FOR THE PREDICTION (1)



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



Example: overfitting due to noisy features

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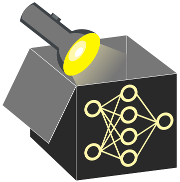

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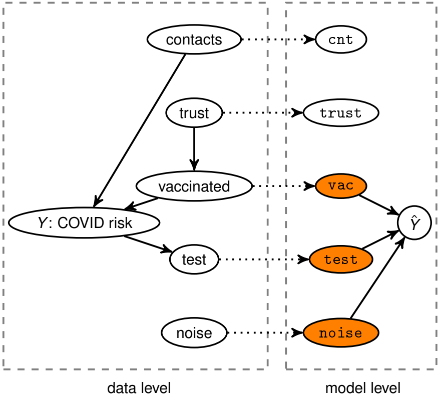


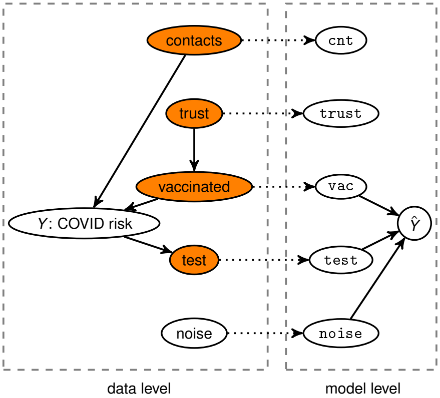
Example: overfitting due to noisy features

- 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)

EXAMPLE: PREDICTION-RELEVANT INFORMATION (2)

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



Example: underfitting, model multiplicity

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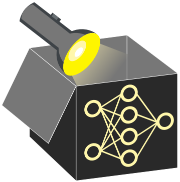

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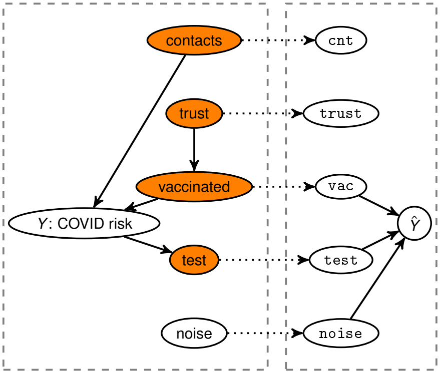


data level   model level

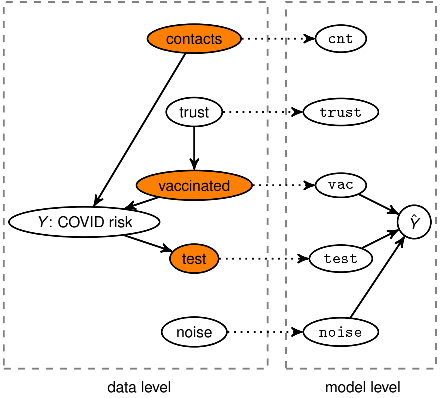
Example: underfitting, model multiplicity

- 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

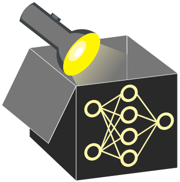
$\Rightarrow$ Underfitted models may ignore prediction-relevant features such as `contacts` here

EXAMPLE: REQUIRES ACCESS TO FEATURE (3)

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



Example: correlations, confounding



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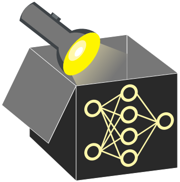

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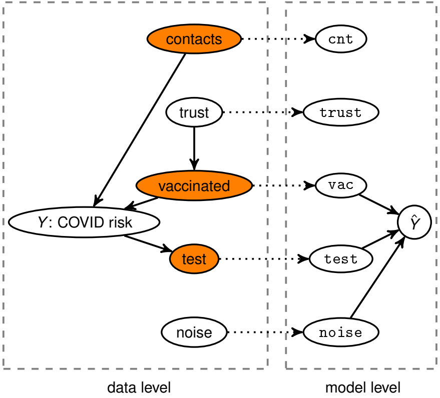

Example: correlations, confounding

- 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

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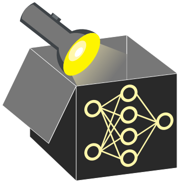

For example, one may be interested in getting insight into whether the ...

(1) feature x_j is causal for the prediction?

- A symptom may help predict a disease ($\leadsto$ causal for $\hat{y}$)
- Intervening on symptom may not affect disease ($\leadsto$ not causal for y)

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

- x_j helps predict y (e.g., conditional expectation) w.r.t. performance
- If $x_j \perp\!\!\!\perp y$, then $\mathbb{E}[y|x_j] = \mathbb{E}[y]$ and x_j and y have 0 mutual info.
  $\leadsto$ x_j carries no prediction-relevant information

(3) model requires access to x_j to achieve its prediction performance?

- x_j helps predict y w.r.t. performance, compared to using only x_{-j}
- If $x_j \perp\!\!\!\perp y|x_{-j}$, then $\mathbb{E}[y|x_{-j}] = \mathbb{E}[y|x_j, x_{-j}]$
  $\leadsto$ 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., if $\mathbb{E}[y \mid x_1] \neq \mathbb{E}[y]$ and $\mathbb{E}[y \mid x_1] = \mathbb{E}[y \mid x_1, x_2]$, a random forest may ignore x_1 in splitting and rely on x_2 instead (despite x_1 being informative).