Interpretable Machine Learning

Introduction to Loss-based Feature Importance

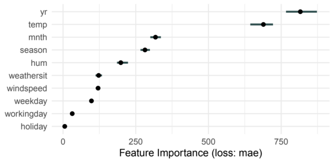


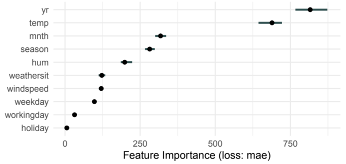
Figure: Bike Sharing Dataset

Learning goals

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

Interpretable Machine Learning

Feature Importances 1
Intro to Loss-based Feature Importance



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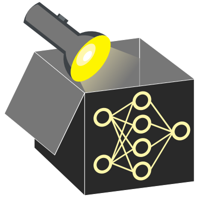

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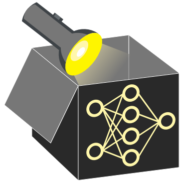

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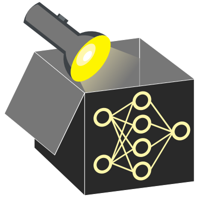

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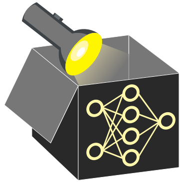

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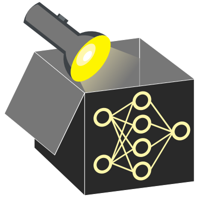

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  $\rightsquigarrow$ Other notions exist (e.g., variance-based methods; see ▸ Greenwell et al. (2020)).

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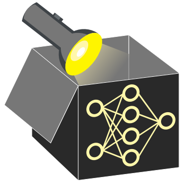

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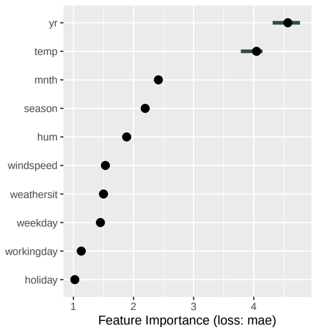
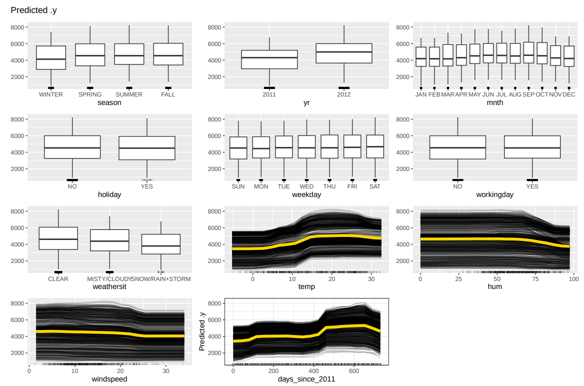
Feature importance offers condensed summary of feat. relevance w.r.t. performance

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





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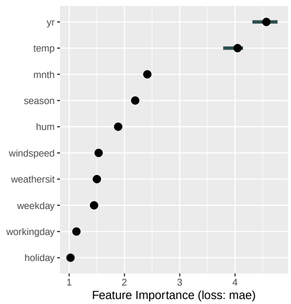
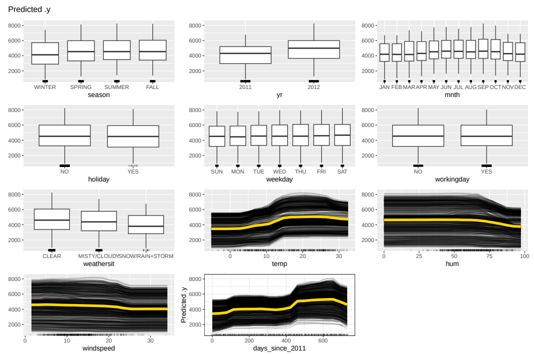
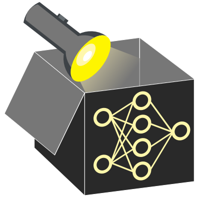




FEATURE IMPORTANCE - DIFFERENCES ▸ Ewald et al. 2024



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* or *conditional* distribution
- **Marginalize X_j:** integrate out X_j via *marginal* or *conditional* distribution

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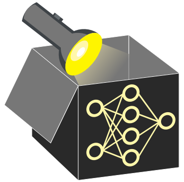

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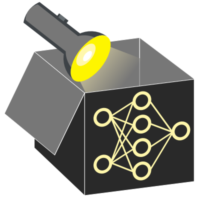

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(2) How they compare model performance before and after feature removal

- **Compare "reduced model" without FOI vs. full model**:
  Measure drop in performance when FOI is "removed"
  ⇝ 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
  ⇝ Similar idea as forward feature selection
- **Compare models with/without FOI across different feature sets**:
  Measure average contribution when FOI joins any feature set (Shapley-based)

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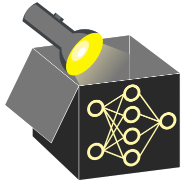

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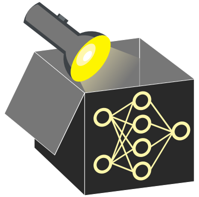

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Depending on the different removal/perturbation and comparison strategies, feature importance methods provide insight into different aspects of model and data.

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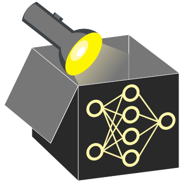

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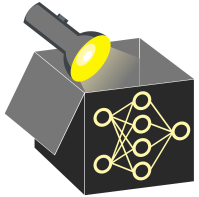

Feature importance methods provide condensed insights, but only into specific aspects of model and data. Interpretation goals often differ and typically address non-overlapping questions (except for special cases).

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

(1) feature x_j is causal for the prediction?

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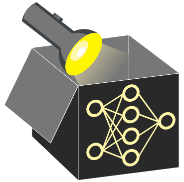

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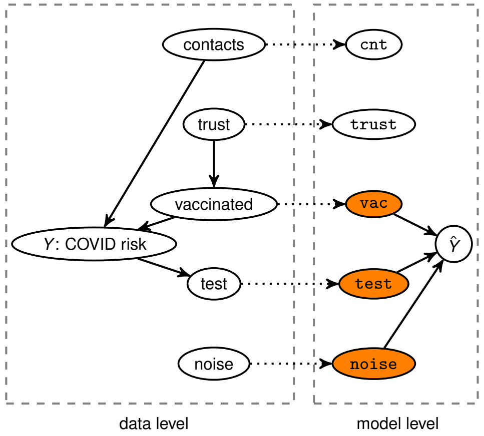
A feature may be causal for $\hat{y}$ (1) without containing prediction-relevant information about y (2)

Example: overfitting due to noisy features



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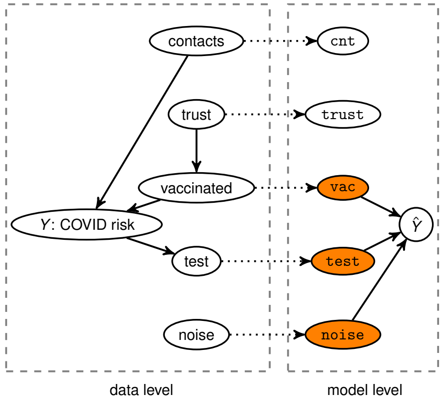

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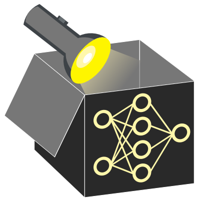

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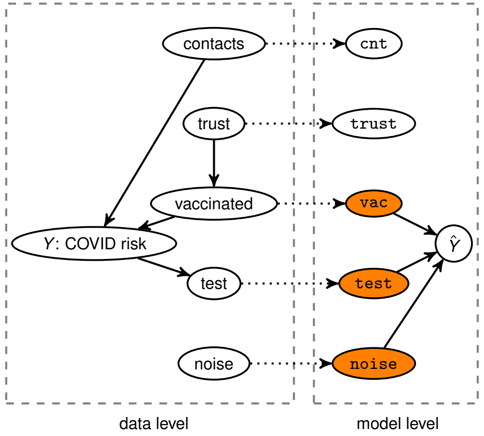

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- All features used by the model are of interest
- Here: Model uses feature `noise`, although it does not contain prediction-relevant information about y (data level)

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

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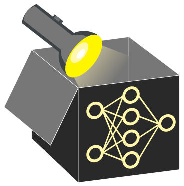

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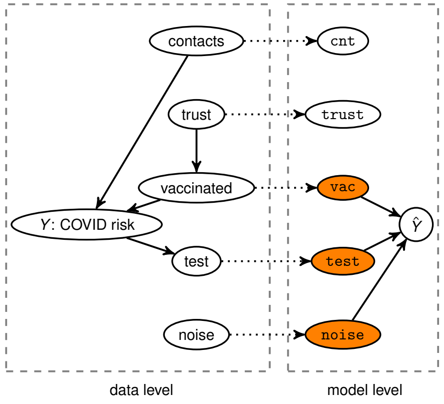

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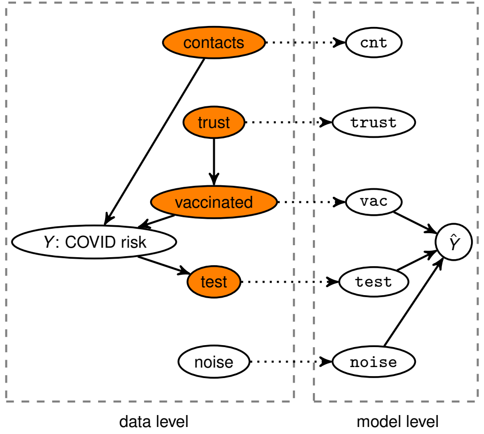
Example: underfitting, model multiplicity



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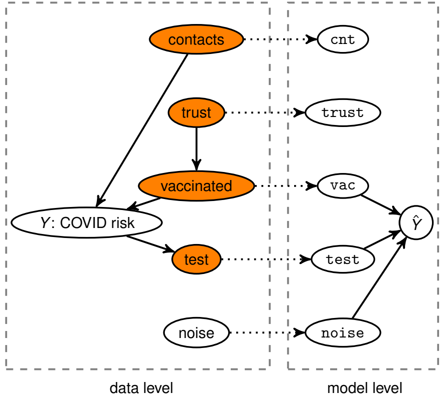

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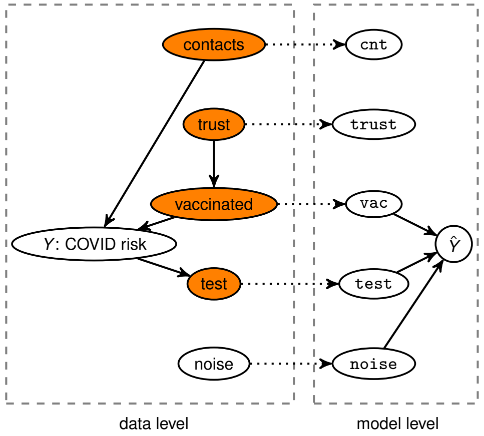

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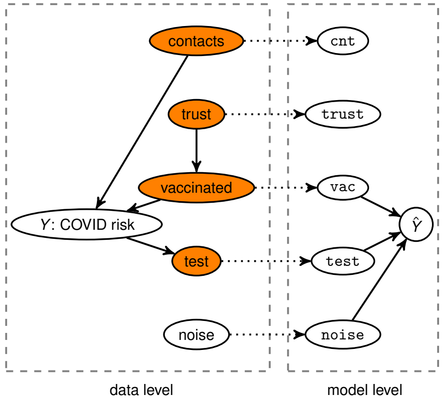

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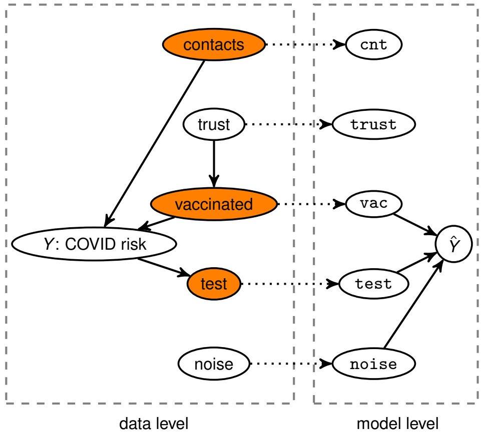

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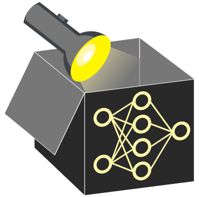

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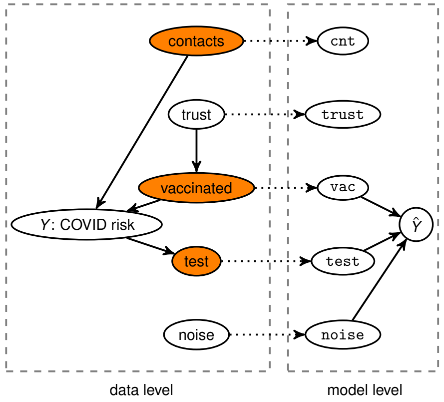

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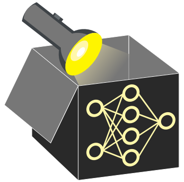

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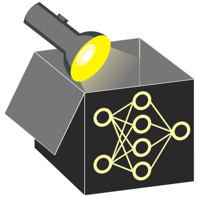

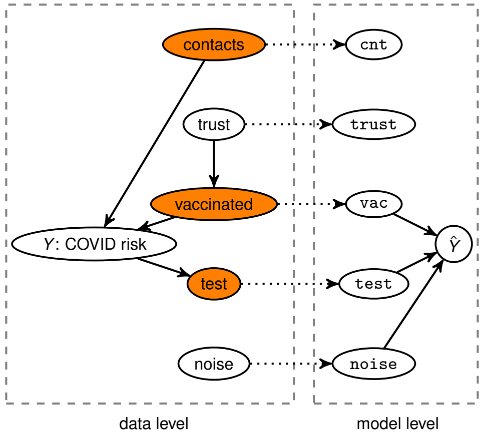

Example: correlations, confounding

- 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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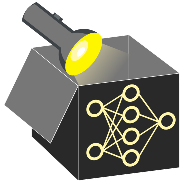

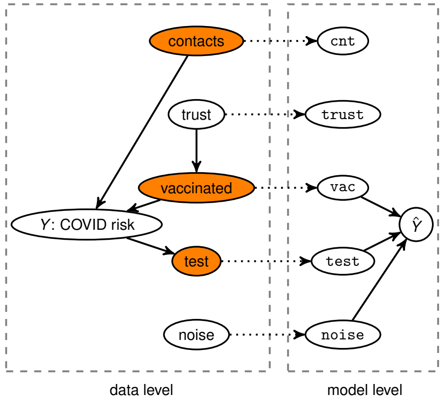

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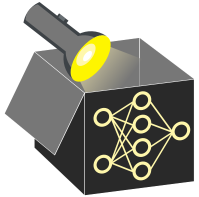


For example, one may be interested in getting insight into whether the ...

(1) feature x_j is causal for the prediction?

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

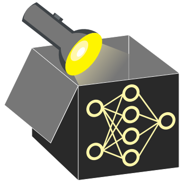
(2) feature x_j contains prediction-relevant information about y?

- 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 zero mutual information
  $\rightsquigarrow$ x_j carries no prediction-relevant information

(3) model requires access to x_j to achieve it's 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 $\mathbb{E}[y|x_{-j}] = \mathbb{E}[y|x_j, x_{-j}]$
  $\rightsquigarrow$ 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., 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).

POTENTIAL INTERPRETATION GOALS



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 ($\rightsquigarrow$ causal for $\hat{y}$)
- Intervening on symptom may not affect disease ($\rightsquigarrow$ 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.
  $\rightsquigarrow$ x_j carries no prediction-relevant information

(3) model requires access to x_j to achieve it's 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 $\mathbb{E}[y|x_{-j}] = \mathbb{E}[y|x_j, x_{-j}]$
  $\rightsquigarrow$ 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., 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).