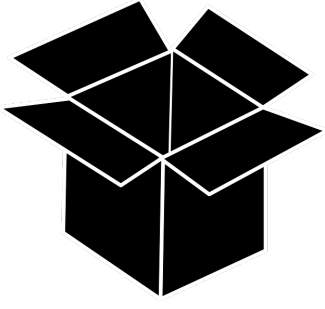
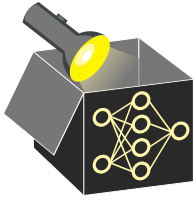
Interpretable Machine Learning

Pitfalls and Best Practices



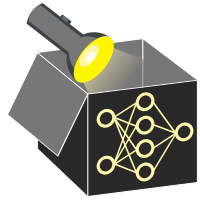


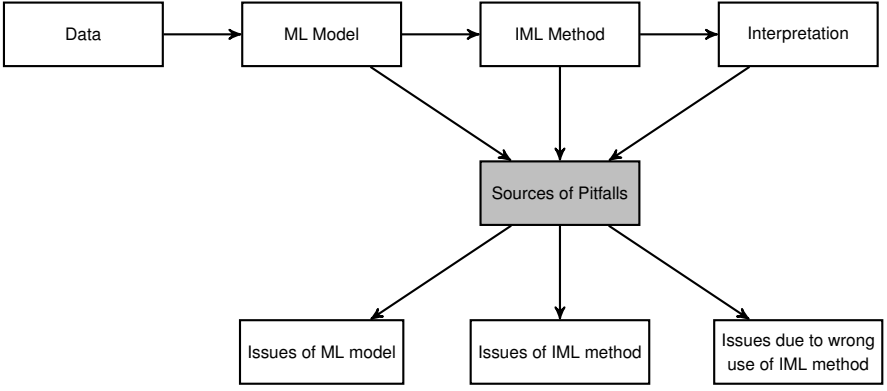
Learning goals

- General pitfalls of interpretation methods
- Practices to avoid pitfalls

SOURCES OF PITFALLS

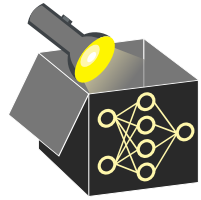
▸ Molnar et. al (2021)





ISSUES OF ML MODEL ▸ Molnar et. al (2021)

- **Proper training and evaluation**: To gain insights into DGP, deployed model should generalize well to unseen data (garbage in, garbage out)



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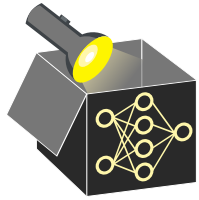

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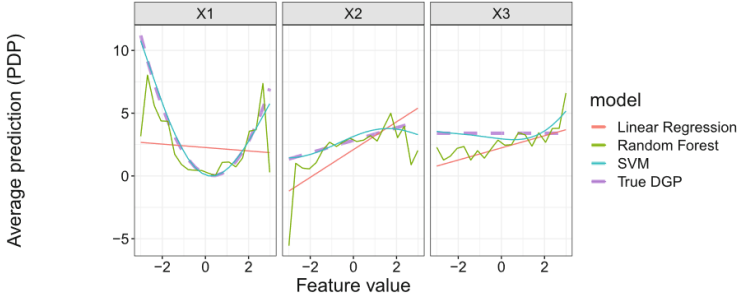
  Example: $X_1, X_2, X_3 \sim Unif(-3, 3)$ with $Y = X_1^2 + X_2 - 5X_1X_2 + \epsilon$, $\epsilon \sim \mathcal{N}(0, 5)$
  Figure: PDP of DGP (true effect), linear regression model (underfitted), random forest (overfitted), and SVM with radial basis kernel (good fit).



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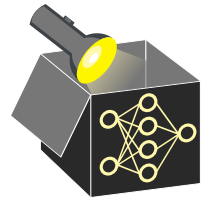

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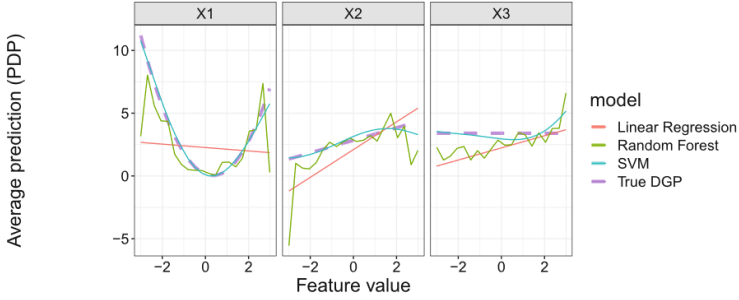

- **Avoid unnecessary complexity**: Prefer simple interpretable models and use them as baseline, move to more complex models if performance not sufficient

ISSUES OF IML METHOD

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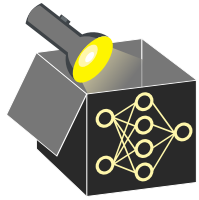
  $\rightsquigarrow$ Check presence of dependencies and use suitable interpretation methods



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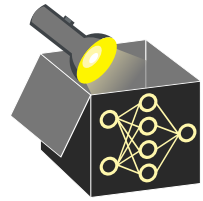

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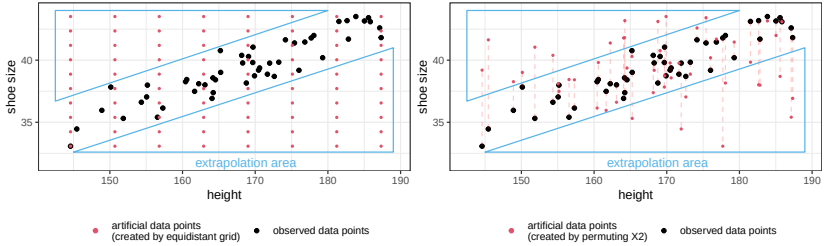

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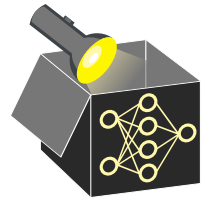

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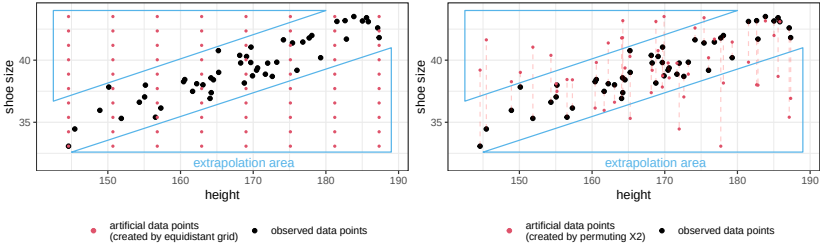
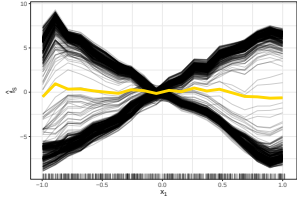
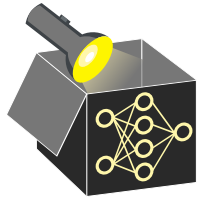


- **Beware of simplifications**: Mapping of complex models to low-dim. explanations
  ⇝ Information loss, e.g., some interpretation methods hide interactions or heterogeneous effects (Figure: PDP and ICE Curves)



INTERPRETATIONS WITH DEPENDENT FEATURES

- Highly correlated features contain similar information
  - ⇝ Model might pick only 1 feat. (regularization), even if it is causally irrelevant
  - ⇝ Produced explanations can be misleading (true to model, but not to data)
  - ⇝ E.g., different interpretable models produce different results



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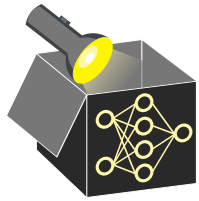

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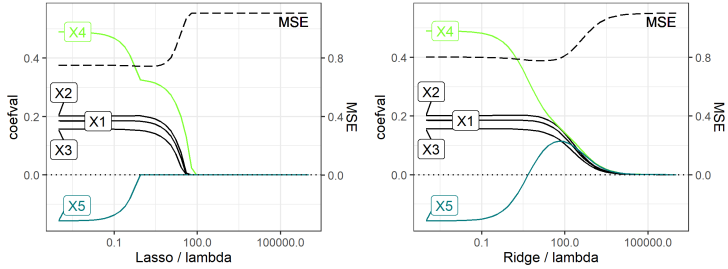
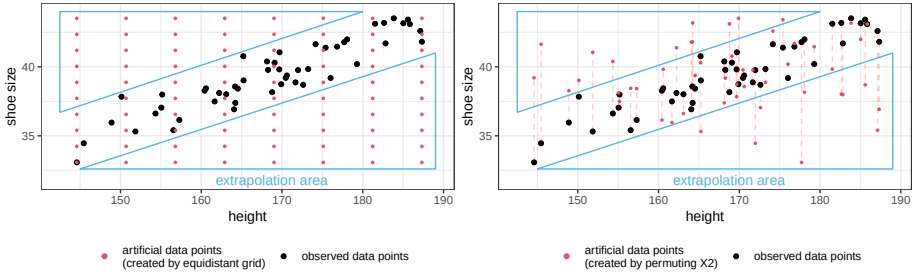
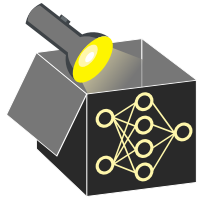
  - $\rightsquigarrow$ E.g., different interpretable models produce different results
- **Example:** Simulate 100 obs. from DGP $Y = 0.2(X_1 + \dots + X_5) + \epsilon, \epsilon \sim N(0, 1)$



- $X_1, \dots, X_4 \sim N(0, 2)$ (uncorrelated)
- $X_5 = X_4 + \delta, \delta \sim N(0, 0.3) \Rightarrow \rho(X_4, X_5) = 0.98$ (highly correlated)
- LASSO: Shrinks coef. of X_5 to zero, coef. of X_4 about $1.5\times$ higher
- Ridge: Similar coef. for X_4 and X_5 for higher lambda

EXTRAPOLATION DUE TO DEPENDENCIES





- Many interpretation methods are based on artificially created data points
  - ⇝ Many points lie in low-density regions if features are dependent
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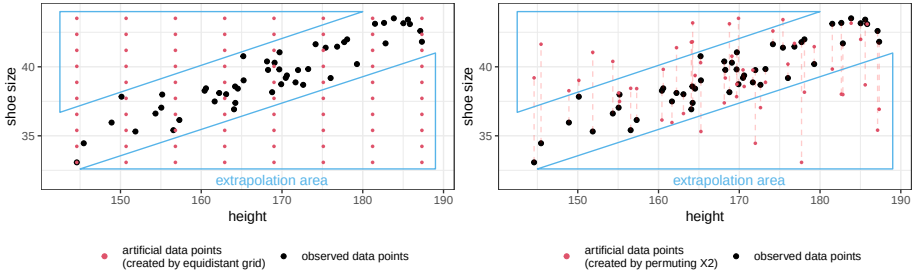

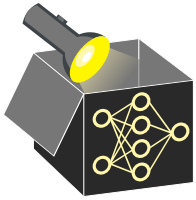

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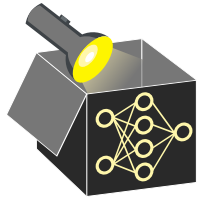
  - ⇝ Many points lie in low-density regions if features are dependent
  - ⇝ Predictions in such regions have high uncertainty
  - ⇝ Explanations can be biased if they rely on pred. where model extrapolated
- There is no definition of when a model extrapolates and to what degree
  - ⇝ Severity of extrapolation depends on model
  - ⇝ Density of train data may helps identify regions where extrapolation is likely
    But: Density estimation in many dimensions is often infeasible

ISSUE: WRONG USE OF IML METHOD

▸ Molnar et. al (2021)

- **Quantify uncertainty**: Interpretation methods are often (statistical) estimators
  $\rightsquigarrow$ Beware of uncertainty, we may need confidence intervals



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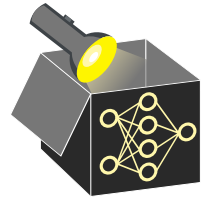

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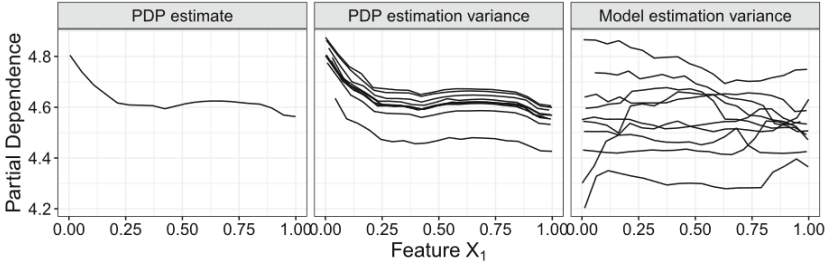

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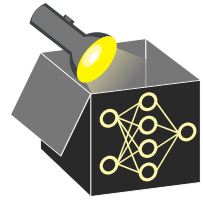

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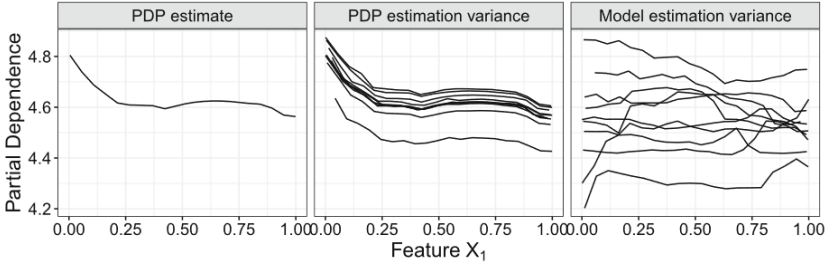

- **Careful with causality**: Want to understand the model or the nature of DGP?
  $\rightsquigarrow$ Goal should guide the choice of interpretation method