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)

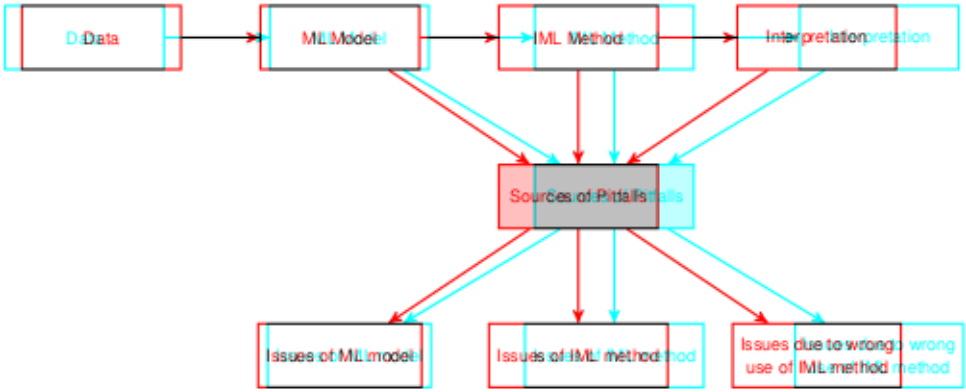

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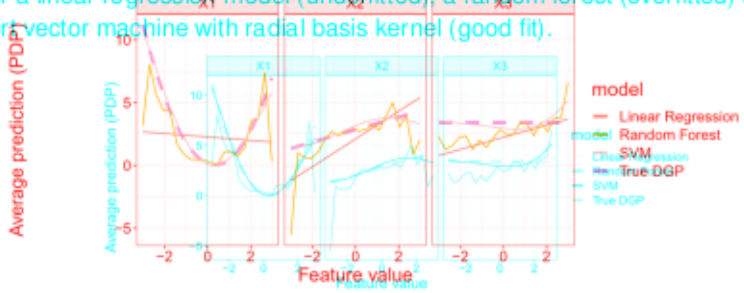
Figure: PDP of DGP (true effect), linear regression model (underfitted), random forest (overfitted), and SVM with radial basis kernel (good fit).

Figure: PDPs for the DGP and for a linear regression model (underfitted), a random forest (overfitted) and a support vector machine with radial basis kernel (good fit).



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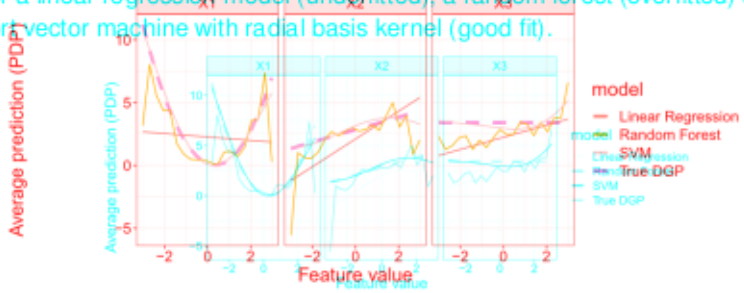

- **Avoid unnecessary complexity**: Prefer simple interpretable models and use them as baseline, move to more complex models if performance not sufficient

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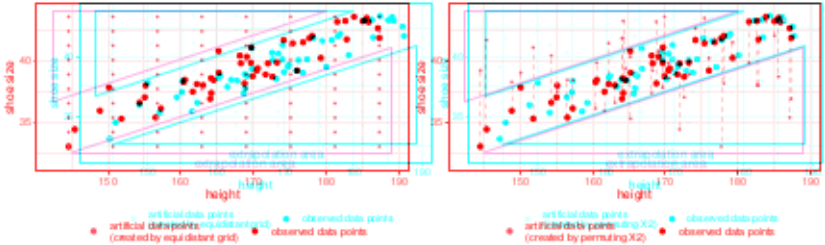

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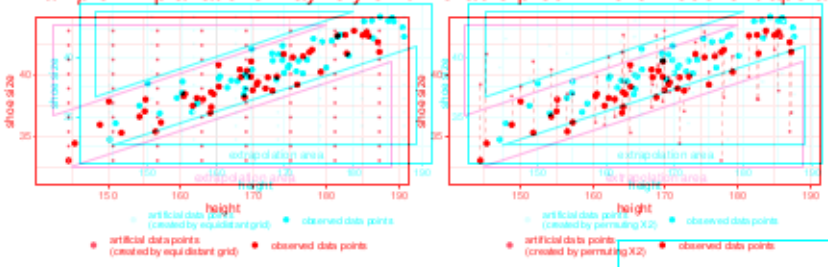
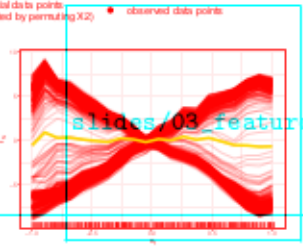


- **Beware of simplifications**: Mapping of complex models to low-dim. explanations
  - ⇝ Information loss, e.g., some interpretation methods hide interactions or heterogeneous effects (Figure: PDP and ICE Curves)



INTERPRETATIONS WITH DEPENDENT FEATURES

METHOD ▸ Molnar et. al (2021)

- 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)
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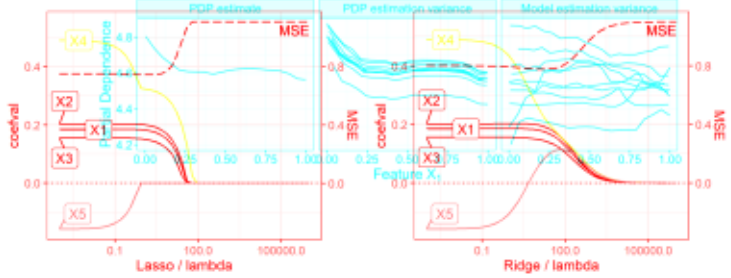
- **Example:** Simulate 100 obs. from DGP $Y = 0.2(X_1 + \dots + X_5) + \epsilon, \epsilon \sim N(0,1)$



- $X_1, \dots, X_4 \sim N(0, 2)$ (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

METHOD

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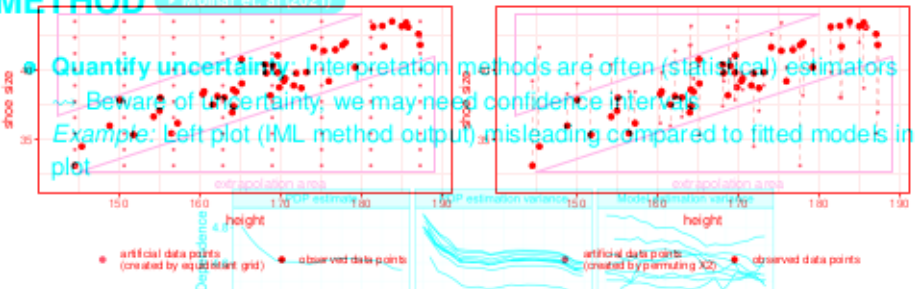

- **Quantify uncertainty:** Interpretation methods are often (statistical) estimators
  - ⇝ Beware of uncertainty: we may need confidence intervals

Example: Left plot (IML method output) misleading compared to fitted models in right plot

- Many interpretation methods are based on artificially created data points
  - ⇝ Many points lie in low-density regions if features are dependent
  - ⇝ Predictions in such regions have high uncertainty
- **Careful with causality:** Do you want to understand the model or the nature of DGP?
  - ⇝ Explanations can be biased if they rely on pred. where model extrapolated
  - ⇝ Your goal should guide the choice of interpretation method