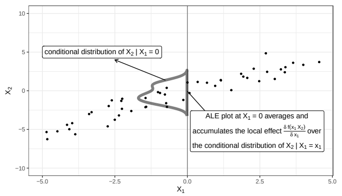
Interpretable Machine Learning

Regional Effects

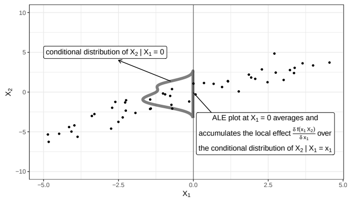


Learning goals

- Difference between feature effects and feature interactions
- REPID

Interpretable Machine Learning

Regional Effects
REPID



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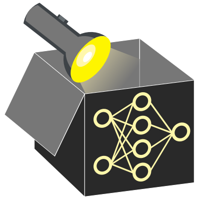
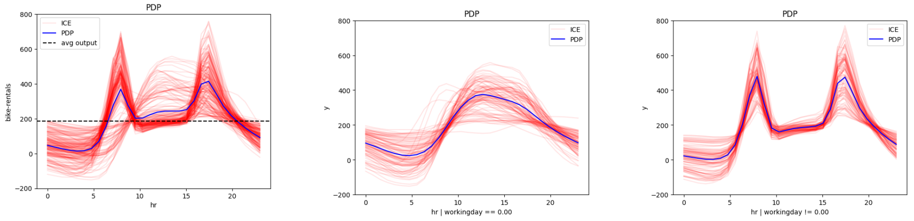
WHY REGIONAL EXPLANATIONS?



Problem: PD & ICE plots can be confounded by feature interactions.
Solution: Group homogeneous ICE curves in such a way that reduces the presence of individual interaction effects within a group $\rightsquigarrow$ Regional effect plots (REPs).

Global Effect	Regional Effect (1)	Regional Effect (2)



- Splitting by the "workingday" revealed 2 different patterns that we're clashed together in the initial plot
- $\cup_i(\texttt{regional\_explanation}_i) = \texttt{global\_explanation}$
- $\textit{Fidelity}(\texttt{regional\_explanation}_i) > \textit{Fidelity}(\texttt{global\_explanation})$

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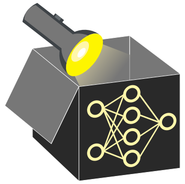

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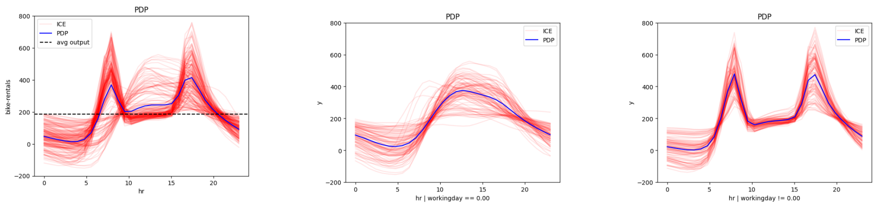

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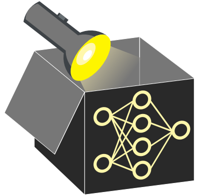

Question: How do feature changes affect the prediction for **one observation**?
Idea: Split $\mathbf{x} = (x_j, \mathbf{x}_{-j})$ into x_j (feature of interest) and $\mathbf{x}_{-j}$ (remaining features)

- Replace observed value x_j with grid values $\tilde{x}_j$ while keeping values $\mathbf{x}_{-j}$ fixed
- Visualize function $\hat{f}(\tilde{x}_j, \mathbf{x}_{-j})$ for varying $\tilde{x}_j$ (ICE)

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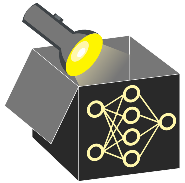

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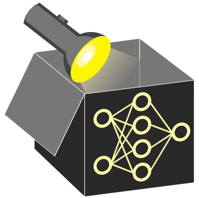

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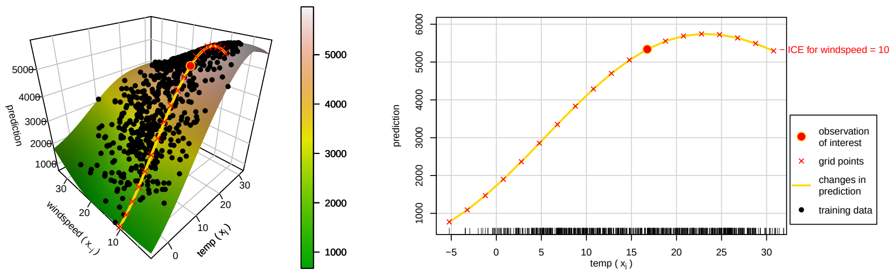
Example: SVM prediction surface (left), select observation and visualize changes in prediction for varying x_2 while keeping x_1 fixed $\Rightarrow$ **local interpretation**



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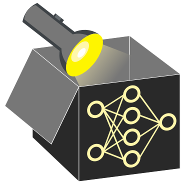

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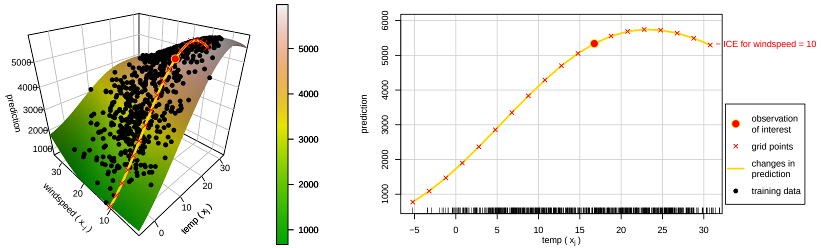
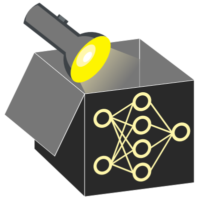


PD PLOT - GLOBAL FEATURE EFFECTS



Question: How do changes of feature values affect model prediction **on average**?

- **PD function**: Integrate out effect of X_{-j} to obtain marginal effect of x_j

$$f_j^{PD}(\tilde{x}_j) = \mathbb{E}_{X_{-j}}[\hat{f}(\tilde{x}_j, X_{-j})] = \int \hat{f}(\tilde{x}_j, X_{-j}) d\mathbb{P}(X_{-j})$$

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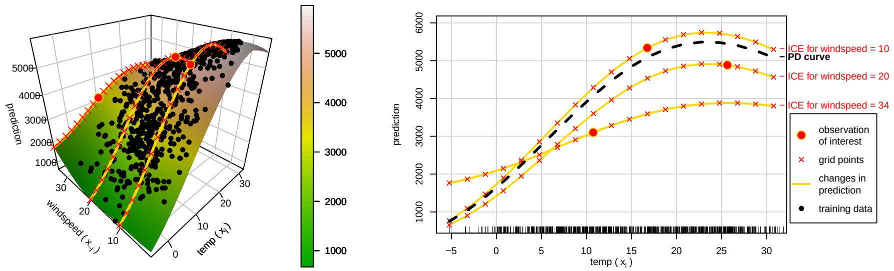

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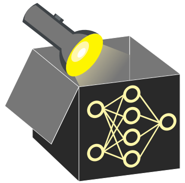

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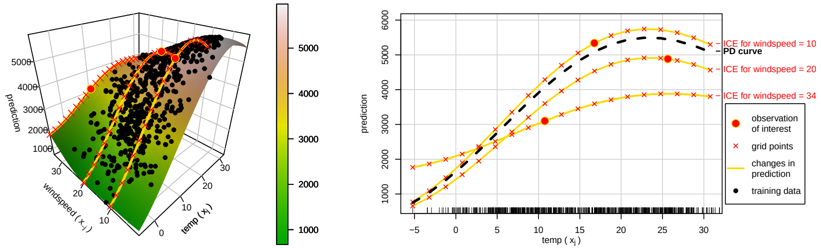
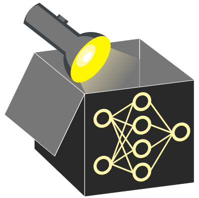


FEATURE INTERACTIONS



Hooker (2004, 2007): Functional ANOVA decomposition of a function

$$\hat{f}(\mathbf{x}) = g_0 + \underbrace{\textstyle\sum_{j=1}^{p} g_j(x_j)}_{\text{main effect}} + \underbrace{\textstyle\sum_{j \neq k} g_{j,k}(x_j, x_k)}_{\text{two-way interaction effect}} + \cdots + \underbrace{g_{1,2,\dots,p}(\mathbf{x})}_{\text{p-way interaction effect}}$$

Friedman and Popescu (2008):

$\Rightarrow$ If x_j and $\mathbf{x}_{-j}$ do not interact, we can decompose $f(\mathbf{x}) = g_j(x_j) + g_{-j}(\mathbf{x}_{-j})$

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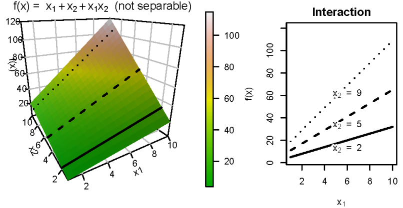
Example: Not additively separable:

$f(\mathbf{x}) = x_1 + x_2 + x_1 \cdot x_2 \neq g(x_1) + g(x_2)$



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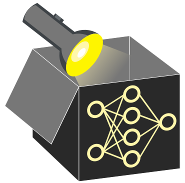

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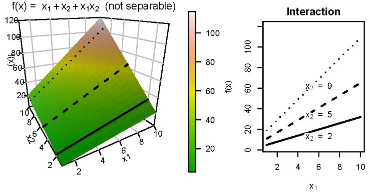

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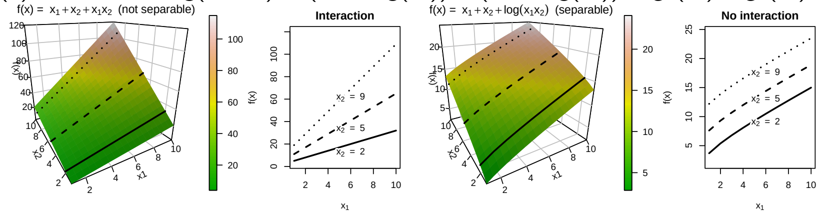

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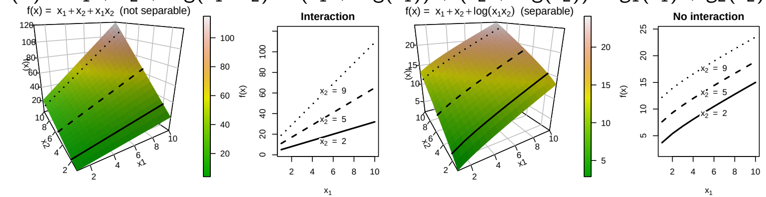

REPID: REGIONAL EFFECT PLOTS ▸ Herbinger et al. (2022)

Recall: Different shapes of ICE curves indicate interactions (ignore vertical shifts)
$\Rightarrow$ Focus on shape differences of **mean-centered ICE curves**.
Mean-centered ICE curve for obs. $\mathbf{x}$ evaluated at m grid points $\tilde{x}_j^{(1)}, \dots, \tilde{x}_j^{(m)}$ is:

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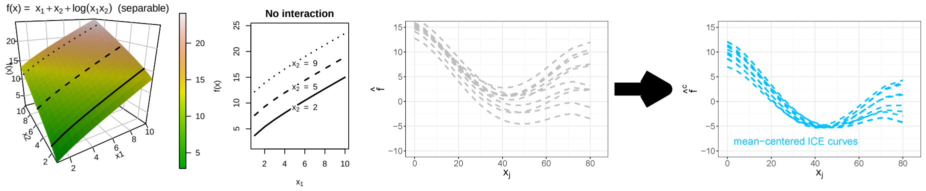

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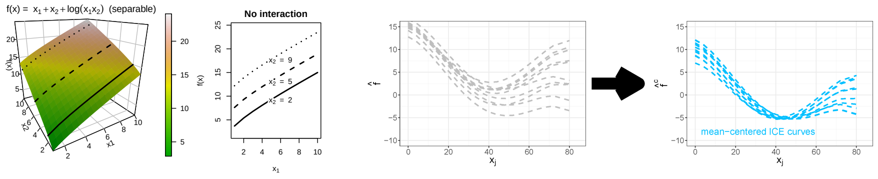


REGIONAL EFFECTS - SYNTHETIC EXAMPLE

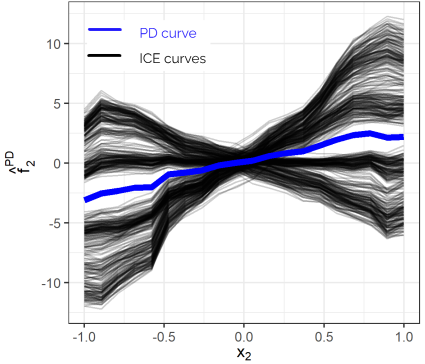
Example: $X_1, X_2, X_6 \sim \mathcal{U}(-1,1)$, $X_3, X_4, X_5 \sim \mathcal{B}(n, 0.5)$ (all iid)

$\rightsquigarrow$ Ground truth: $f(X) = 0.2X_1 \boxed{-8X_2 + 8X_2\mathbb{1}_{(X_1>0)} + 16X_2\mathbb{1}_{(X_3=0)}} + \epsilon$

$\rightsquigarrow$ Model: Random forest

Problem:

- PD curve of $\boxed{X_2}$ is misleading due to interactions $\rightsquigarrow$ ICE
- ICE curves do not identify the interacting features



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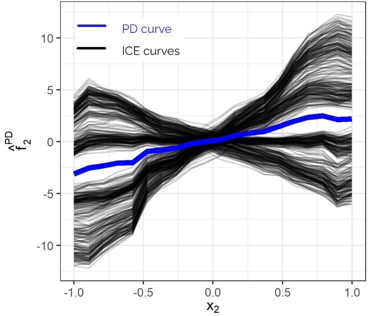

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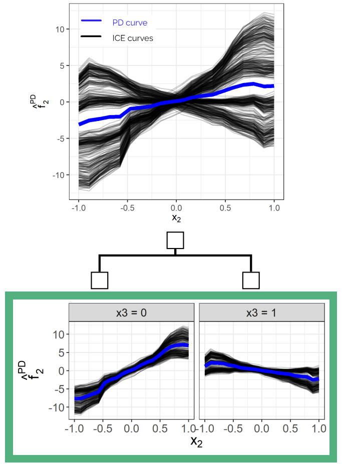

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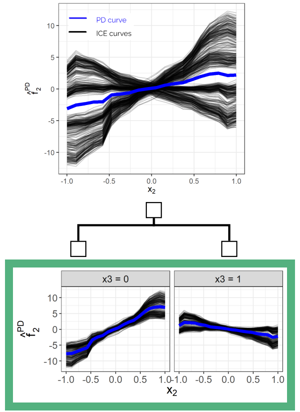

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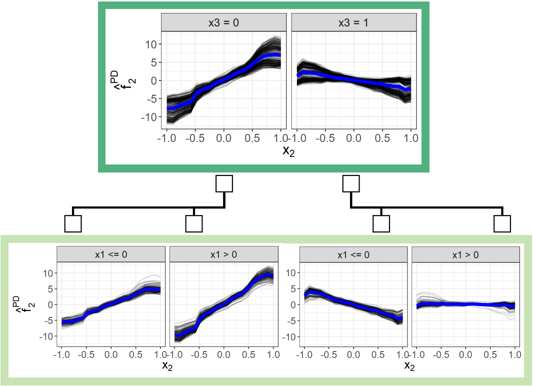
Regional effect (blue curves) $\hat{=}$ Estimate PD curve in each region



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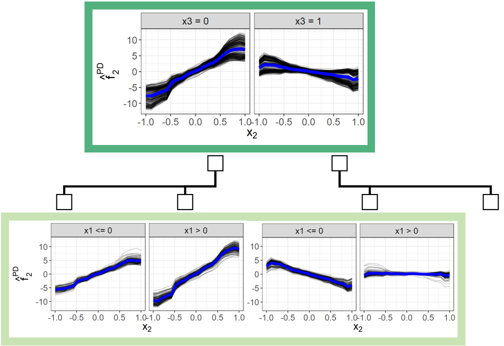

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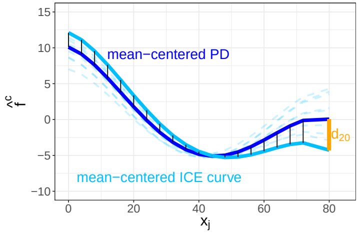
REGIONAL EFFECTS - DETAILS

Question: How to split the curves into regions?
Define risk as L2 loss of mean-centered ICE curves:

$$\mathcal{R}_j(\mathcal{N}) = \sum_{\mathbf{x} \in \mathcal{N}} \sum_{k=1}^{m} \underbrace{\left(\hat{f}^c(\tilde{x}_j^{(k)}, \mathbf{x}_{-j}) - \hat{f}^{PD,c}_{j|\mathcal{N}}(\tilde{x}_j^{(k)})\right)^2}_{d_k}$$



with the average feature effect in region $\mathcal{N} \subseteq \mathcal{X}$:

$$\hat{f}^{PD,c}_{j|\mathcal{N}}(\tilde{x}_j) = \frac{1}{|\mathcal{N}|} \sum_{\mathbf{x} \in \mathcal{N}} \hat{f}^c(\tilde{x}_j, \mathbf{x}_{-j})$$

$\Rightarrow$ Measures interaction-related heterogeneity (variance) of ICE curves in $\mathcal{N}$

$\Rightarrow$ Recursive partitioning (CART): Find best feature-split combination that solves

$$\arg\min_{z,t} \; \mathcal{R}_j(\mathcal{N}_{left}) + \mathcal{R}_j(\mathcal{N}_{right})$$

- $\mathcal{N}_{left} = \{\mathbf{x} \in \mathcal{N} | x_z \leq t\}$
- $\mathcal{N}_{right} = \{\mathbf{x} \in \mathcal{N} | x_z > t\}$
- Split point t for feature $x_z, z \in -j$

Intuition: Is another feature x_z responsible for the heterogeneity (measured by $\mathcal{R}_j$)?

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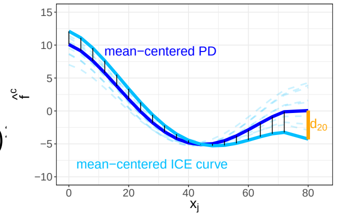


with the avg. feature effect in region $\mathcal{N} \subseteq \mathcal{X}$:

$$\hat{f}^{PD,c}_{j|\mathcal{N}}(\tilde{x}_j) = \frac{1}{|\mathcal{N}|} \sum_{\mathbf{x} \in \mathcal{N}} \hat{f}^c(\tilde{x}_j, \mathbf{x}_{-j})$$

$\leadsto$ Measures interaction-related heterogeneity (variance) of ICE curves in $\mathcal{N}$

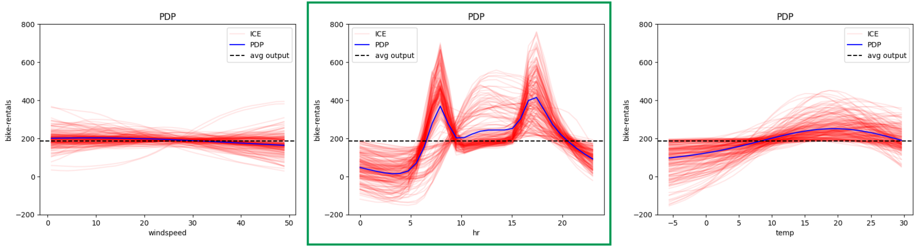
$\leadsto$ Recursive partitioning (CART): Find best feat-split combo that solves

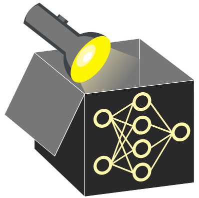
$$\arg\min_{z,t} \; \mathcal{R}_j(\mathcal{N}_{left}) + \mathcal{R}_j(\mathcal{N}_{right})$$

- $\mathcal{N}_{left} = \{\mathbf{x} \in \mathcal{N} | x_z \leq t\}$
- $\mathcal{N}_{right} = \{\mathbf{x} \in \mathcal{N} | x_z > t\}$
- Split point t for feature $x_z, z \in -j$

Intuition: Is another feature x_z responsible for the heterogeneity (measured by $\mathcal{R}_j$)?

REGIONAL EFFECT PLOTS - REAL EXAMPLE





- Identify feature with highly heterogeneous local effects
  ⇝ `hour`: Most important and highly heterogeneous feature (highest variance)
- Find regions in feature space where this heterogeneity is minimal
  ⇝ Partition feature space using CART to minimize variance of mean-centered ICE curves within each region

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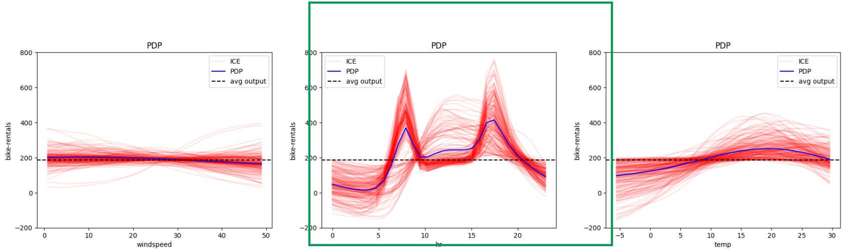

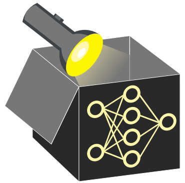

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Interpretable Machine Learning – 8 / 9

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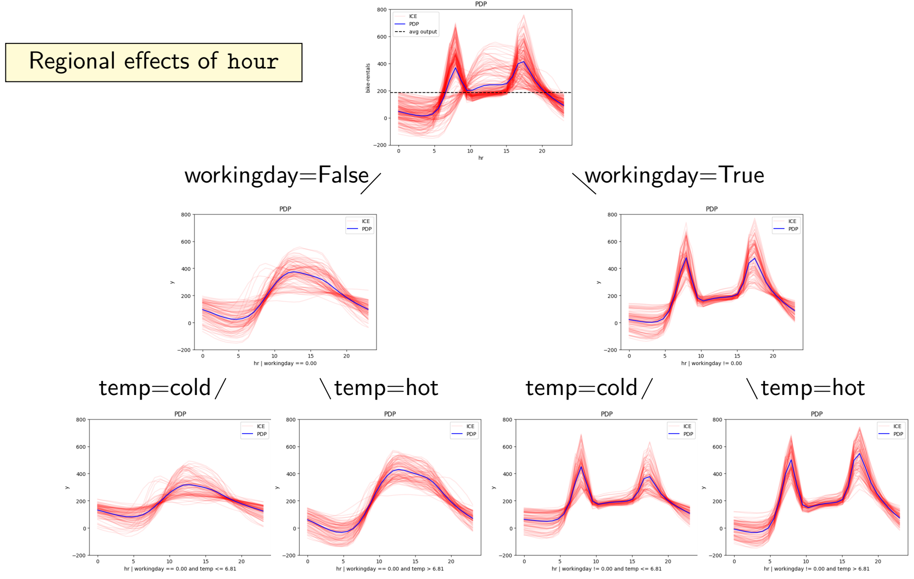

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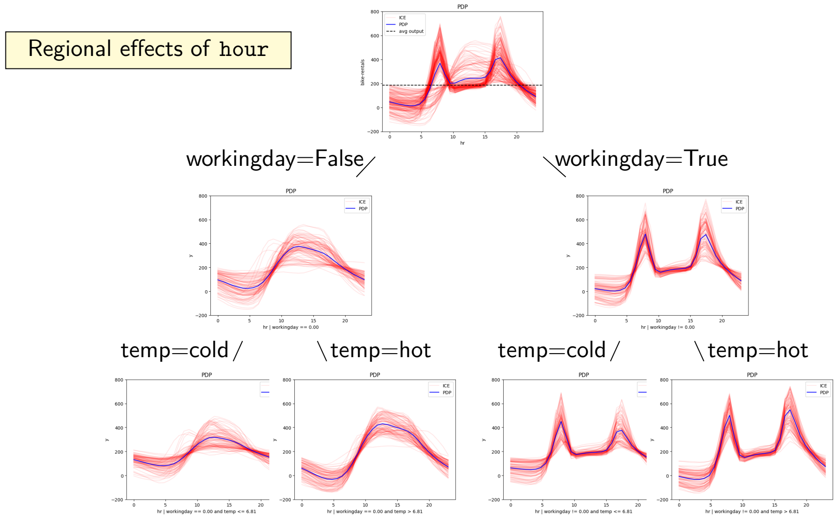
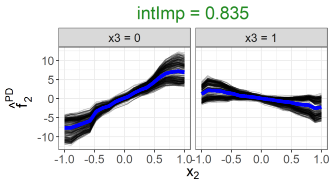


Interpretable Machine Learning

Regional Effects



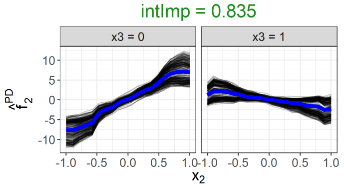
Learning goals

- Interaction quantification
- REPID interaction importance

Interpretable Machine Learning

Regional Effects

Interaction importance



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INTERACTION QUANTIFICATION

It's helpful to know not just how another feature changes the marginal effect of x_S but how strong that interaction is and want to rank features by it.

Approaches:

- **H-Statistics:** Variance of the deviation between the joint PDP and the sum of marginal PDPs (larger variance $\Rightarrow$ stronger interaction).
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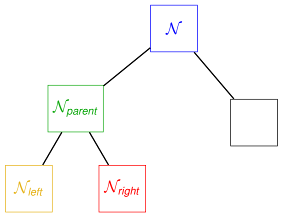
On parent node level (for $\mathcal{N}_{parent}$):

$$intImp(\mathcal{N}_{parent}) = \frac{\mathcal{R}(\mathcal{N}_{parent}) - (\mathcal{R}(\mathcal{N}_{left}) + \mathcal{R}(\mathcal{N}_{right}))}{\mathcal{R}(\mathcal{N})}$$

Interpretation: Reduction of ICE curve variance after one split of $\mathcal{N}_{parent}$ into $\mathcal{N}_{left}$ and $\mathcal{N}_{right}$ relative to the ICE curve variance in the root node $\mathcal{N}$.



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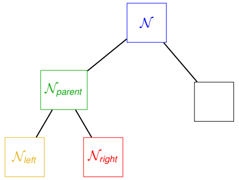

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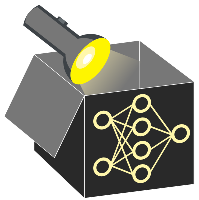

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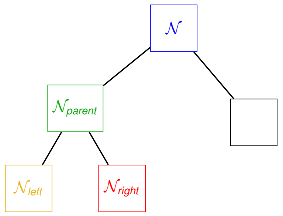

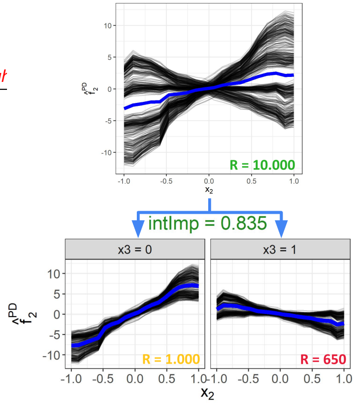

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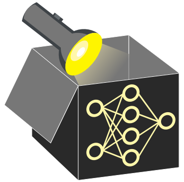

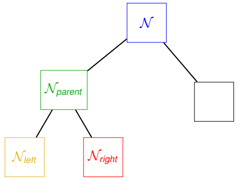

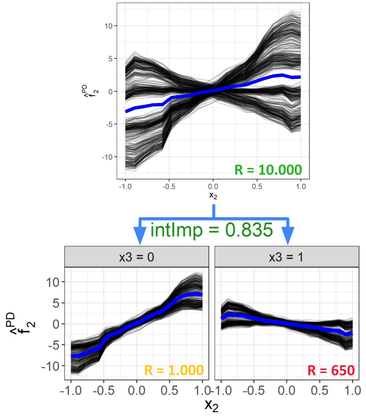

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Interpretable Machine Learning – 2 / 8

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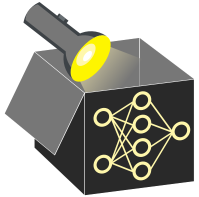

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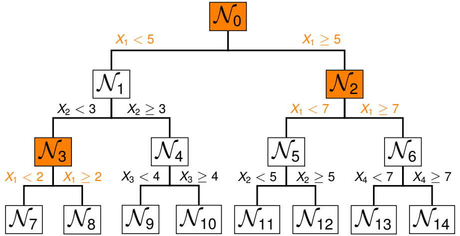
Example: For $X_1 \Rightarrow \mathcal{B}_1 = \{0, 2, 3\}$



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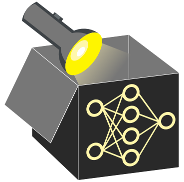

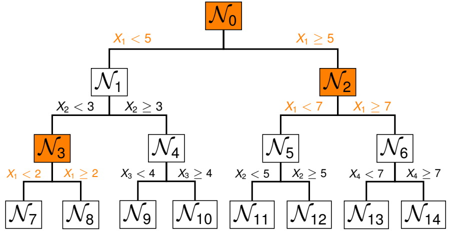

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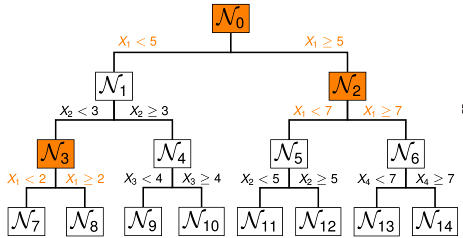

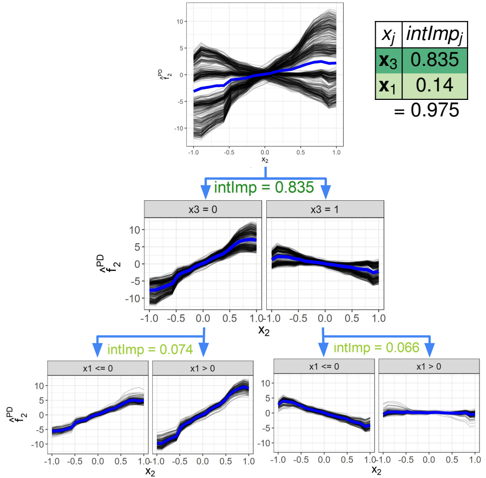

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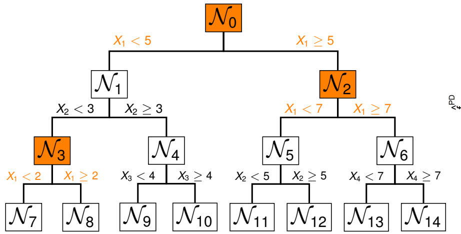

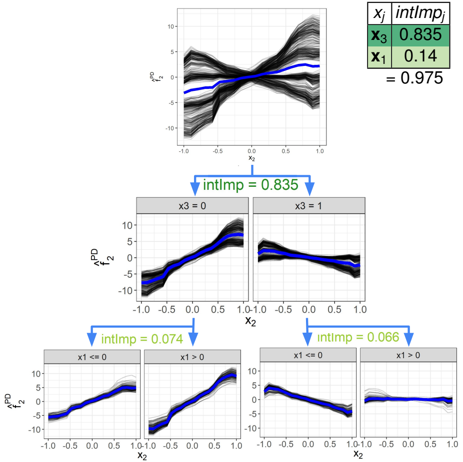

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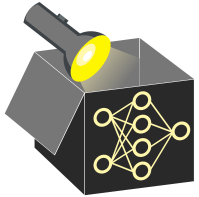
Interpretable Machine Learning – 3 / 8

OUTPERFORMING SOTA



Simulation setting

- Draw 1000 i.i.d. samples from $X_1, \dots, X_4 \sim \mathcal{U}(-1, 1)$
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- 30 repetitions, measure interaction strength between $\mathbf{x}_2$ and all other 3 features

Which methods are sensitive to changes in main effect sizes or feature correlations?

Pitfall	REPID	H-Statistic	Greenwell	SHAP
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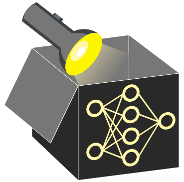

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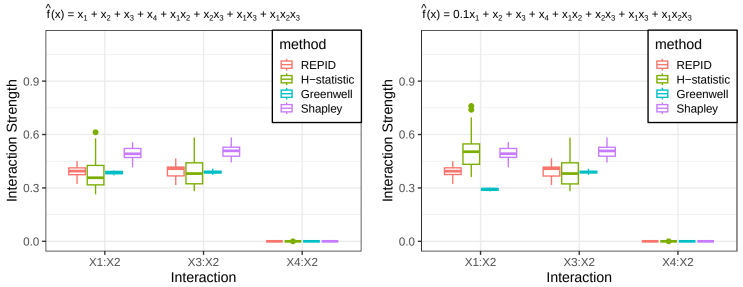

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  - **Expectation**: Interaction strengths should not change
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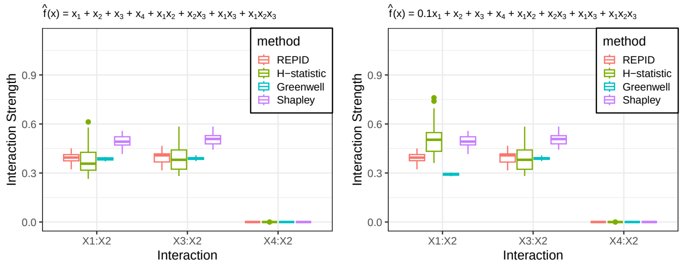
OUTPERFORMING SOTA



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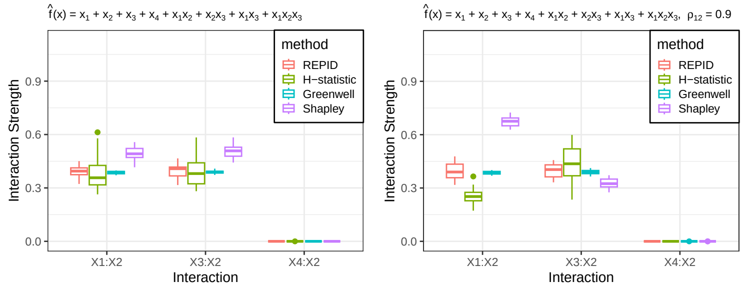

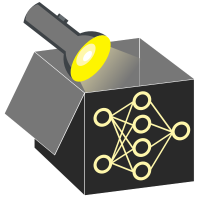

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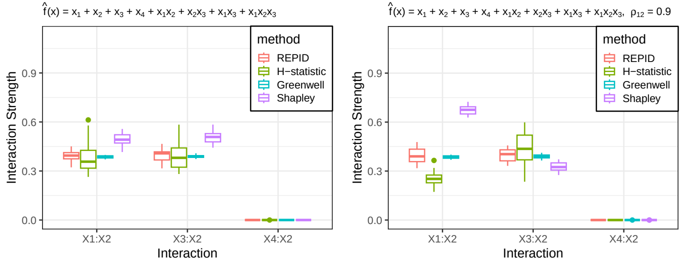

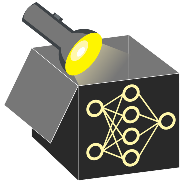

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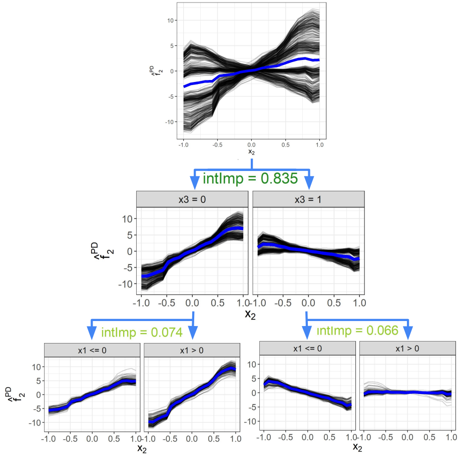
$\Rightarrow$ Different regions for different features



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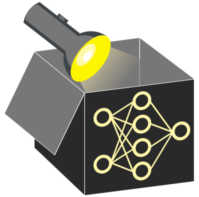

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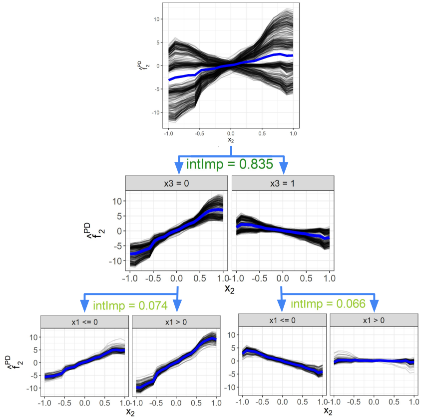

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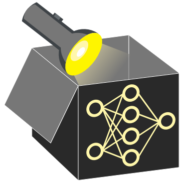


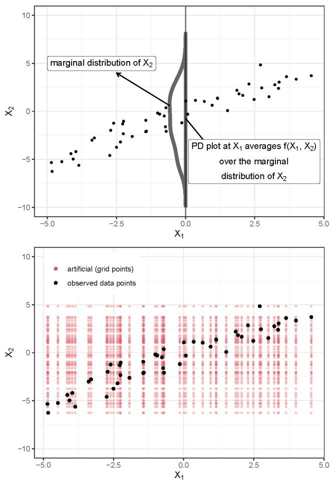
Interpretable Machine Learning – 7 / 8

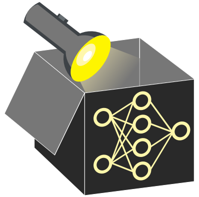
LIMITATIONS OF REPID

1) Restricted to one feature of interest
⇒ Different regions for different features

2) Restricted to PD (global) and ICE (local) as feature effect methods
⇒ Inherits extrapolation problem (unlikely combinations of feature values)

⇝ Follow-up GADGET [under review]





LIMITATIONS OF REPID

1) Restricted to one feature of interest
⇒ Different regions for different features

2) Restricted to PD (global) and ICE (local) as feature effect methods
⇒ Inherits extrapolation problem (unlikely combinations of feature values)

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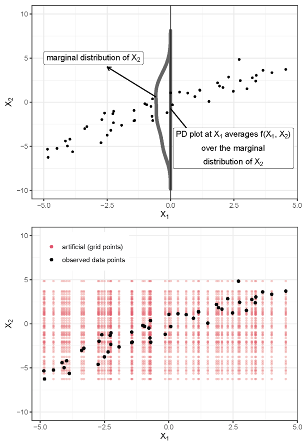
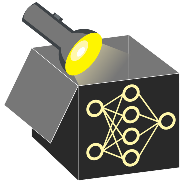




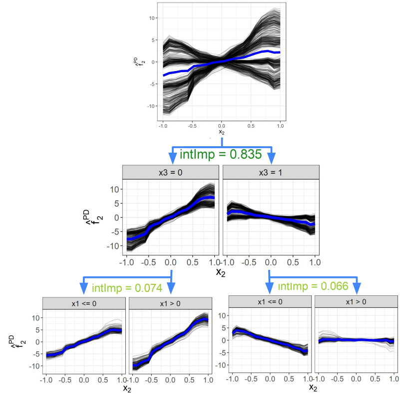
CONCLUSION

Summary of Contributions (REPID):

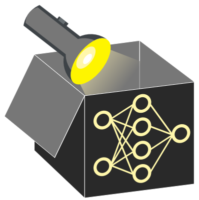
- Regional effects in interpretable regions
- Additive decomposition of feature effect
- Quantify feature interactions
- Outperforms SOTA interaction indices

Summary of Contributions (GADGET):

- Unique regions for multiple features
- Additive decomposition of prediction function
- Extension to ALE and Shapley Dependence
- Test to identify significant interactions



$\hat{f}_2^{PD}(X_2) \approx 8X_2 \quad \approx 16X_2 \quad \approx -8X_2 \quad \approx 0$



Further Directions:
Pruning, GADGET as a predictor, comparing regions across models, efficient implementation, more efficient testing and splitting approach, . . .

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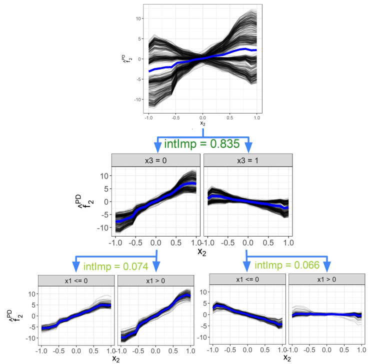

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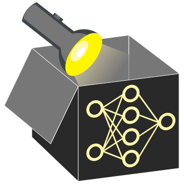

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