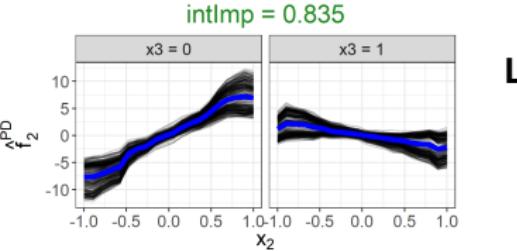


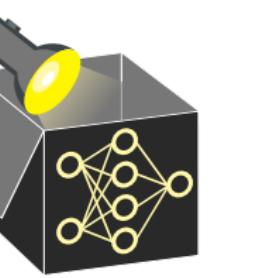
Interpretable Machine Learning

Regional Effects



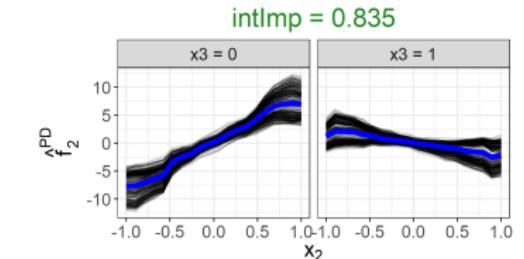
Learning goals

- Interaction quantification
- REPID interaction importance



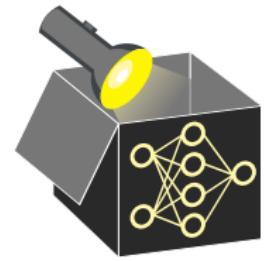
Interpretable Machine Learning

Regional Effects Interaction importance



Learning goals

- Interaction quantification
- REPID interaction importance

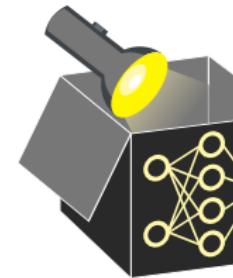


INTERACTION QUANTIFICATION

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).
- **Greenwell's Interaction Index:** Difference between the variance of the PDP and the mean variance of centered ICE curves for the same feature pair.
- **SHAP interaction index** ([▶ Herbinger et al. \(2022\)](#), [▶ Lundberg et al. 2018](#)): Proportion of all two-way interactions with x_i to which the j -th feature contributes.

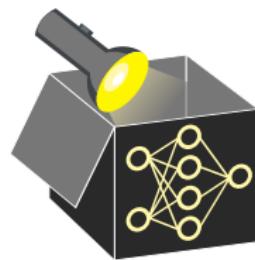


INTERACTION QUANTIFICATION

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).
- **Greenwell's Interaction Index:** Difference between variance of the PDP and the mean variance of centered ICE curves for the same feature pair.
- **SHAP interaction index** ([▶ Herbinger 2022](#), [▶ Lundberg 2018](#)): Proportion of all two-way interactions with x_i to which the j -th feature contributes.



INTERACTION QUANTIFICATION

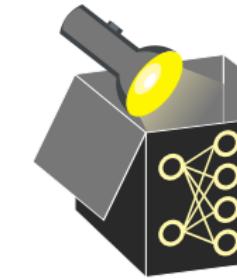
It's helpful to know not just how another feature changes the marginal effect of x_S but how strong that interaction is and want to rank features by it.

Approaches:

- **H-Statistics:** Variance of the deviation between the joint PDP and the sum of marginal PDPs (larger variance \Rightarrow stronger interaction).
- **Greenwell's Interaction Index:** Difference between the variance of the PDP and the mean variance of centered ICE curves for the same feature pair.
- **SHAP interaction index** ([▶ Herbinger et al. \(2022\)](#), [▶ Lundberg et al. 2018](#)): Proportion of all two-way interactions with x_i to which the j -th feature contributes.

Pitfalls:

- The values of H-Statistic and the Greenwell's Interaction Index are influenced by the main effects of the two regarded features.
- SHAP interaction index does not suffer from main effect problem. However, correlation between the two features can bias the interaction value. Same applies to the H-Statistic.



INTERACTION QUANTIFICATION

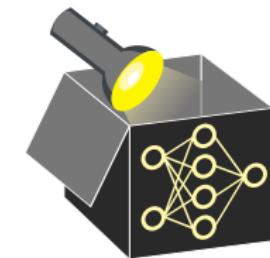
It's helpful to know not just how another feature changes the marginal effect of x_S but how strong that interaction is and want to rank features by it.

Approaches:

- **H-Statistics:** Variance of the deviation between the joint PDP and the sum of marginal PDPs (larger variance \Rightarrow stronger interaction).
- **Greenwell's Interaction Index:** Difference between variance of the PDP and the mean variance of centered ICE curves for the same feature pair.
- **SHAP interaction index** ([▶ Herbinger 2022](#), [▶ Lundberg 2018](#)): Proportion of all two-way interactions with x_i to which the j -th feature contributes.

Pitfalls:

- The values of H-Statistic and the Greenwell's Interaction Index are influenced by the main effects of the two regarded features.
- SHAP interaction index does not suffer from main effect problem. However, correlation between the two features can bias the interaction value. Same applies to the H-Statistic.

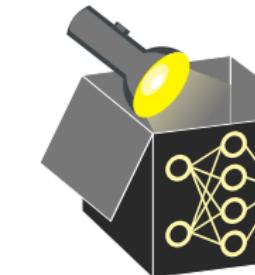
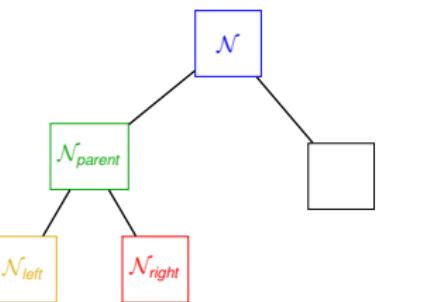


REPID INTERACTION IMPORTANCE

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} .

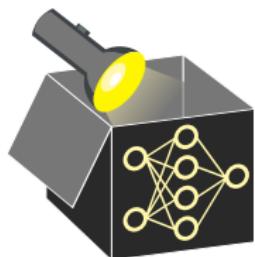
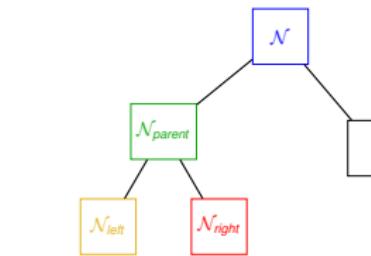


REPID INTERACTION IMPORTANCE

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} .

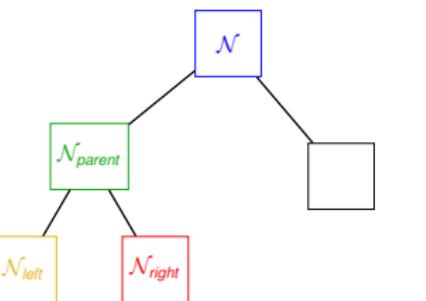


REPID INTERACTION IMPORTANCE

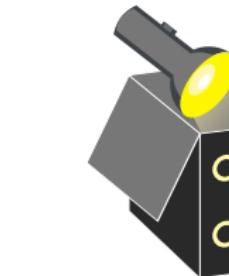
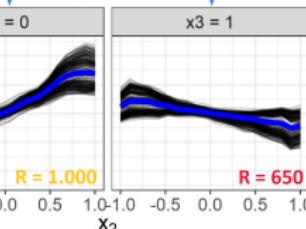
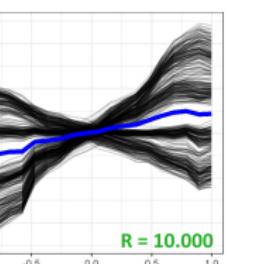
On parent node level (for \mathcal{N}_{parent}):

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

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} .



Split reduces 83.5% of variance.

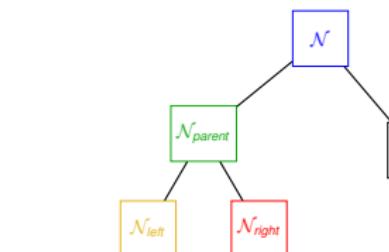


REPID INTERACTION IMPORTANCE

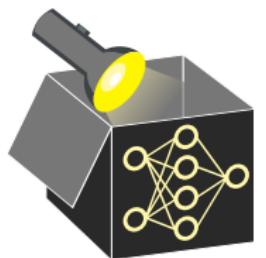
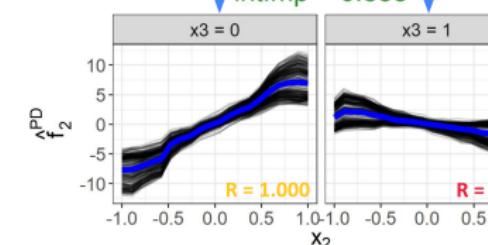
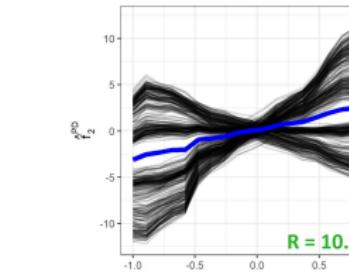
On parent node level (for \mathcal{N}_{parent}):

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

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} .



Split reduces 83.5% of variance.



REPID INTERACTION IMPORTANCE

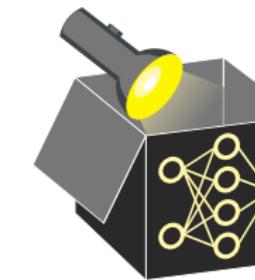
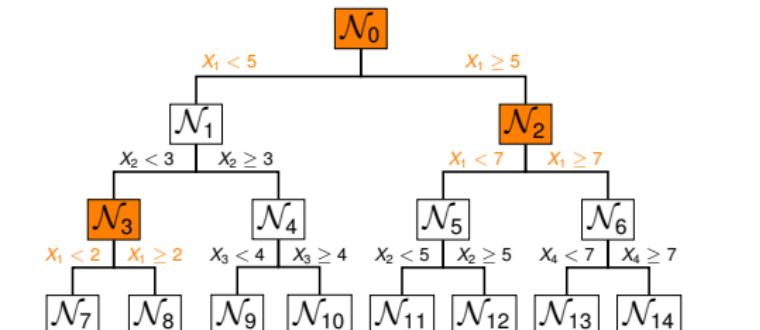
On feature level (for x_j):

$$intImp_j = \sum_{i \in \mathcal{B}_j} intImp(\mathcal{N}_i)$$

where \mathcal{B}_j indexes parent nodes split by x_j .

Interpretation: Overall reduction of ICE curve variance due to splits by X_j (in %).

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



REPID INTERACTION IMPORTANCE

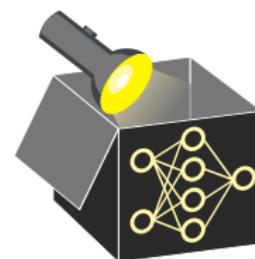
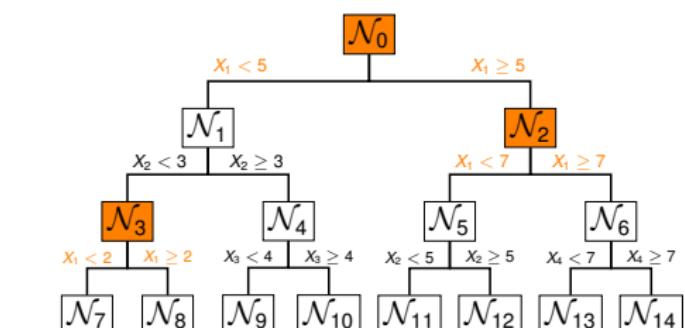
On feature level (for x_j):

$$intImp_j = \sum_{i \in \mathcal{B}_j} intImp(\mathcal{N}_i)$$

where \mathcal{B}_j indexes parent nodes split by x_j .

Interpretation: Overall reduction of ICE curve variance due to splits by X_j (in %).

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



REPID INTERACTION IMPORTANCE

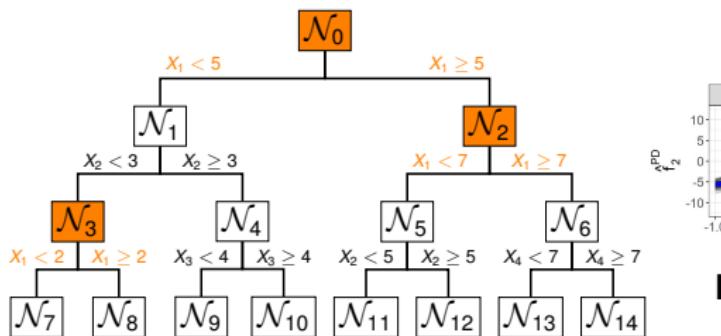
On feature level (for x_j):

$$intImp_j = \sum_{i \in \mathcal{B}_j} intImp(\mathcal{N}_i)$$

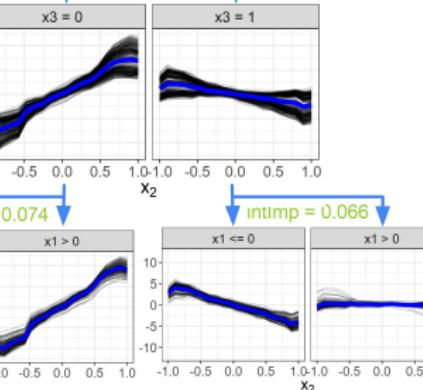
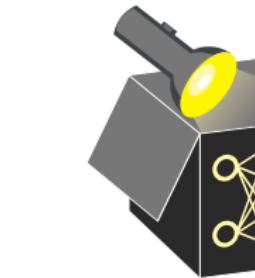
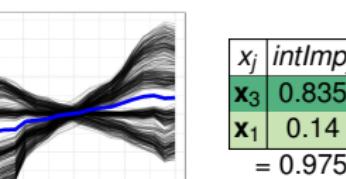
where \mathcal{B}_j indexes parent nodes split by x_j .

Interpretation: Overall reduction of ICE curve variance due to splits by X_j (in %).

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



Note: $intImp$ can also be used as a stopping criterion.



REPID INTERACTION IMPORTANCE

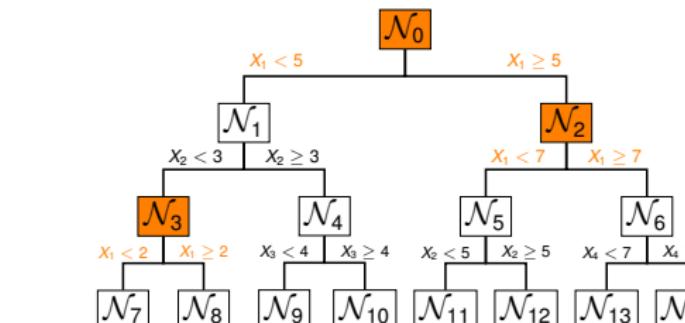
On feature level (for x_j):

$$intImp_j = \sum_{i \in \mathcal{B}_j} intImp(\mathcal{N}_i)$$

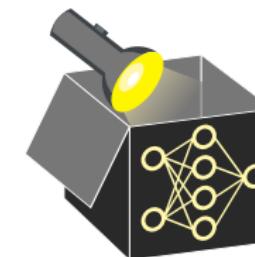
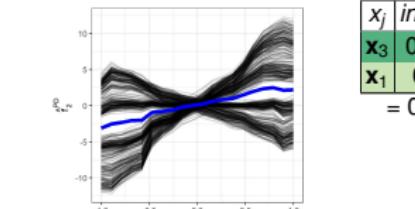
where \mathcal{B}_j indexes parent nodes split by x_j .

Interpretation: Overall reduction of ICE curve variance due to splits by X_j (in %).

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



Note: $intImp$ can also be used as a stopping criterion.

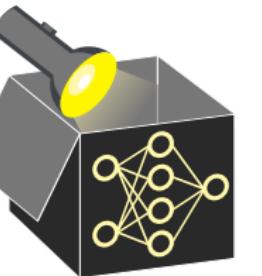


OUTPERFORMING SOTA

Simulation setting

- Draw 1000 i.i.d. samples from $X_1, \dots, X_4 \sim \mathcal{U}(-1, 1)$
- True underlying function: $f(\mathbf{x}) = \sum_{j=1}^4 \mathbf{x}_j + \mathbf{x}_1\mathbf{x}_2 + \mathbf{x}_2\mathbf{x}_3 + \mathbf{x}_1\mathbf{x}_3 + \mathbf{x}_1\mathbf{x}_2\mathbf{x}_3 + \epsilon$
- Fit a correctly specified linear model (interactions with \mathbf{x}_4 are excluded)
- 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
sensitive to changes of main effect	No	Yes	Yes	No
sensitive to changes of correlation between \mathbf{x}_j and other features	No	Yes	No	Yes

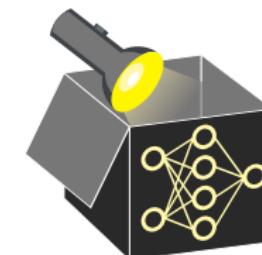
OUTPERFORMING SOTA

Simulation setting

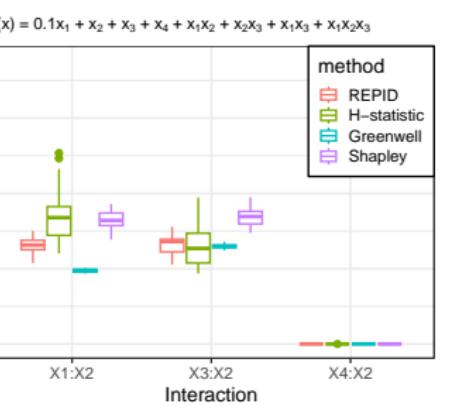
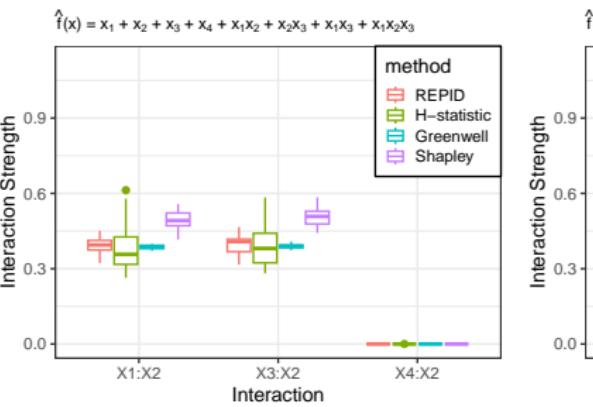
- Draw 1000 i.i.d. samples from $X_1, \dots, X_4 \sim \mathcal{U}(-1, 1)$
- True underlying function:
$$f(\mathbf{x}) = \sum_{j=1}^4 \mathbf{x}_j + \mathbf{x}_1\mathbf{x}_2 + \mathbf{x}_2\mathbf{x}_3 + \mathbf{x}_1\mathbf{x}_3 + \mathbf{x}_1\mathbf{x}_2\mathbf{x}_3 + \epsilon$$
- Fit a correctly specified linear model (interactions with \mathbf{x}_4 are excluded)
- 30 reps, 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?

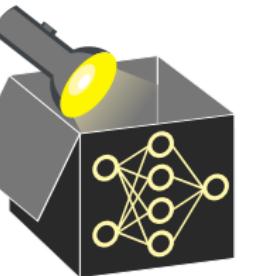
Pitfall	REPID	H-Statistic	Greenwell	SHAP
sensitive to changes of main effect	No	Yes	Yes	No
sensitive to changes of correlation between \mathbf{x}_j and other features	No	Yes	No	Yes



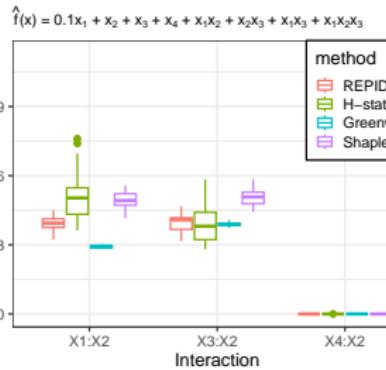
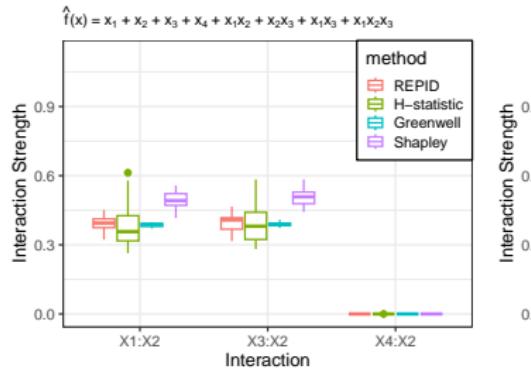
OUTPERFORMING SOTA



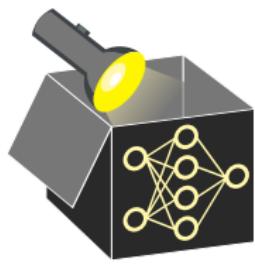
- **Left (initial setting):** Interaction strength of $x_1:x_2$ and $x_3:x_2$ similar; $x_4:x_2$ no interaction
- **Right:** Set main effect $\beta_1 = 0.1$
 - **Expectation:** Interaction strengths should not change
 - **Fail:** H-statistic ($x_1:x_2 > x_3:x_2$) and Greenwell ($x_1:x_2 < x_3:x_2$)



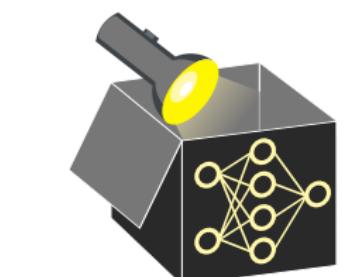
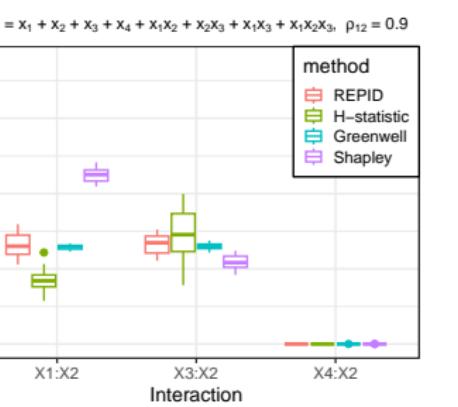
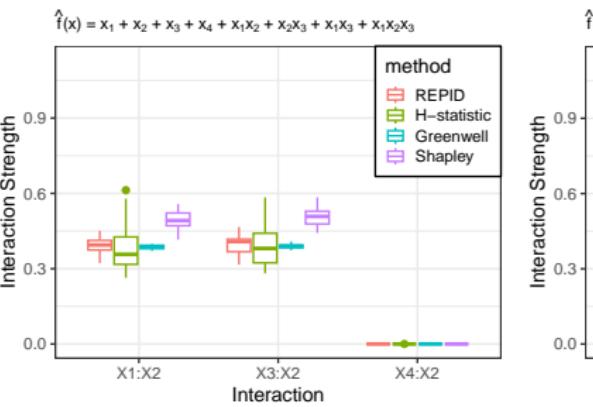
OUTPERFORMING SOTA



- **Left (initial setting):** Interaction strength of $x_1:x_2$ and $x_3:x_2$ similar; $x_4:x_2$ no interaction
- **Right:** Set main effect $\beta_1 = 0.1$
 - **Expectation:** Interaction strengths should not change
 - **Fail:** H-statistic ($x_1:x_2 > x_3:x_2$) and Greenwell ($x_1:x_2 < x_3:x_2$)

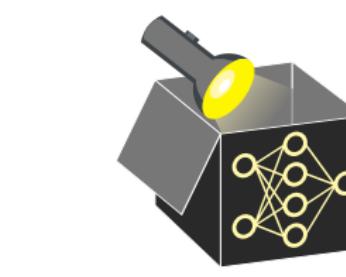
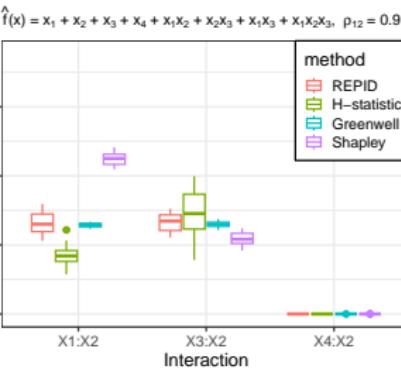
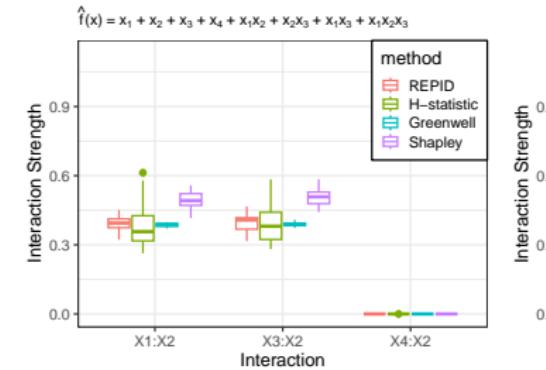


OUTPERFORMING SOTA



- **Left (initial setting):** Interaction strength of $x_1:x_2$ and $x_3:x_2$ similar; $x_4:x_2$ no interaction
- **Right:** Increase correlation $\rho(x_1, x_2) = 0.9$
 - **Expectation:** Interaction strengths should not change
 - **Fail:** H-statistic ($x_1:x_2 < x_3:x_2$) and Shapley ($x_1:x_2 > x_3:x_2$)
- **REPID is the only method which always leads to correct rankings for these settings**

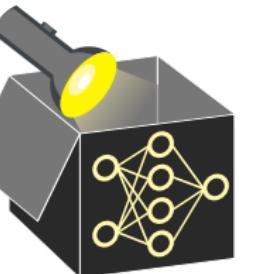
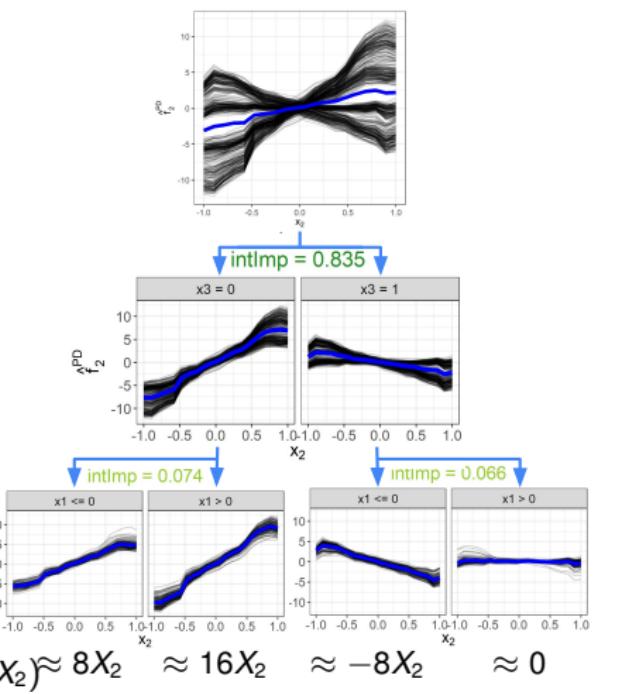
OUTPERFORMING SOTA



- **Left (initial setting):** Interaction strength of $x_1:x_2$ and $x_3:x_2$ similar; $x_4:x_2$ no interaction
- **Right:** Increase correlation $\rho(x_1, x_2) = 0.9$
 - **Expectation:** Interaction strengths should not change
 - **Fail:** H-statistic ($x_1:x_2 < x_3:x_2$) and Shapley ($x_1:x_2 > x_3:x_2$)
- **REPID is the only method which always leads to correct rankings for these settings**

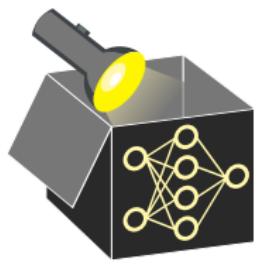
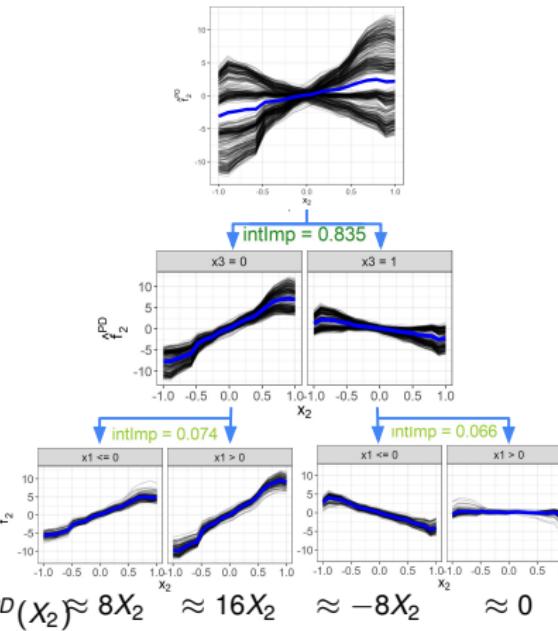
LIMITATIONS OF REPID

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



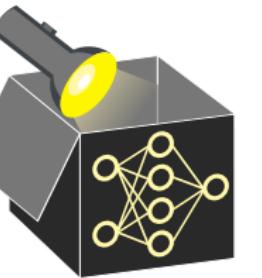
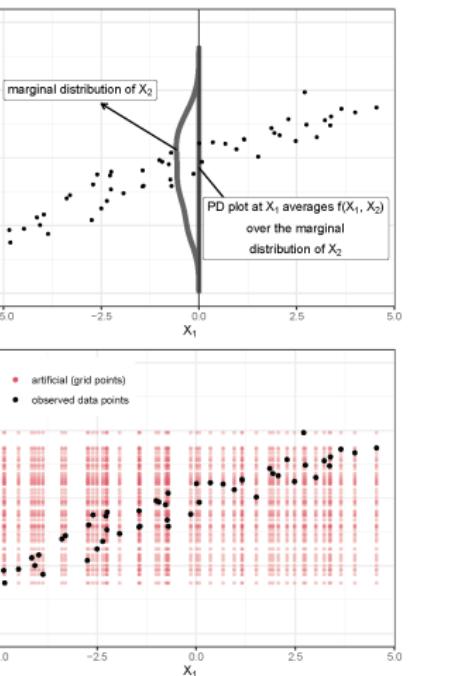
LIMITATIONS OF REPID

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



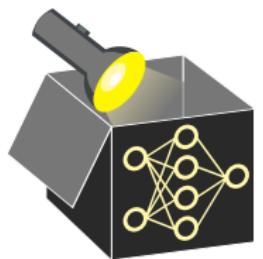
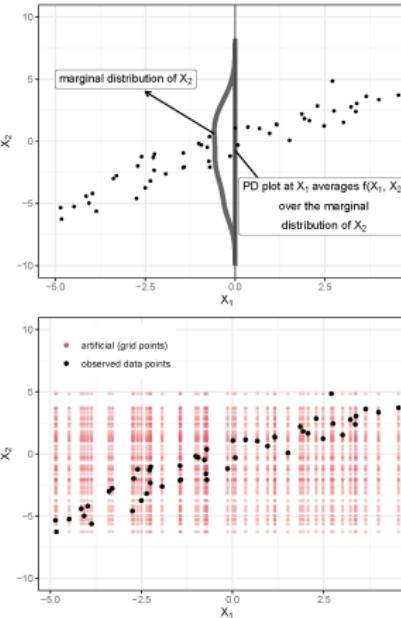
LIMITATIONS OF REPID

- 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)
- ~~ Follow-up GADGET [under review]



CONCLUSION

Summary of Contributions (REPID):

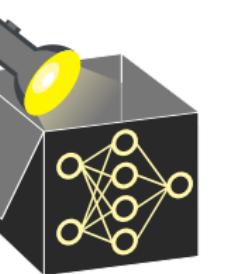
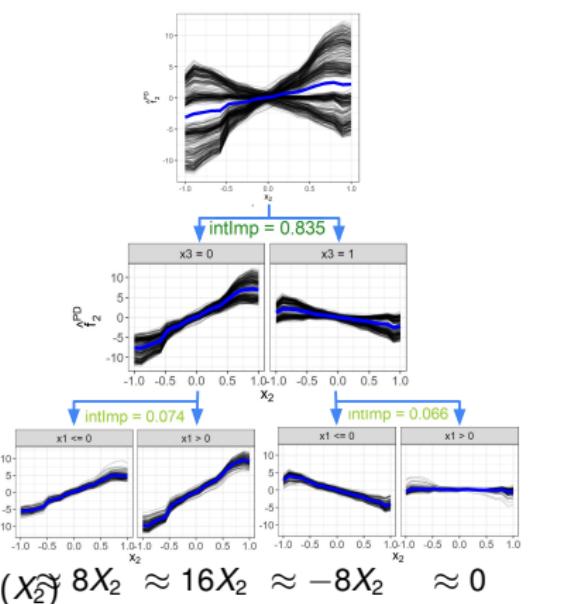
- Regional effects in interpretable regions
- Additive decomposition of feature effect
- Quantify feature interactions
- Outperforms SOTA interaction indices

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

Further Directions:

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



CONCLUSION

Summary of Contributions (REPID):

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

Summary of Contributions (GADGET):

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

Further Directions:

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

