

Random Planted Forest

A Directly Interpretable Tree Ensemble

Meyer, J. T.⁵ Burk, L.^{1,2,3,4} Hiabu, M.⁶ Mammen, E.⁵

¹Leibniz Institute for Prevention Research and Epidemiology – BIPS

²LMU Munich ³University of Bremen

⁴Munich Center for Machine Learning (MCML)

⁵Heidelberg University ⁶University of Copenhagen

Motivation



1

- Individual decision trees: Easy to interpret

Random Planted Forest (RPF): Additive Random Forest

Motivation



1

- Individual decision trees: Easy to interpret
- Random Forest (RF): Less so

Random Planted Forest (RPF): Additive Random Forest

Motivation



1

- Individual decision trees: Easy to interpret
- Random Forest (RF): Less so
- **Desirable properties:**

Random Planted Forest (RPF): Additive Random Forest

Motivation



1

- Individual decision trees: Easy to interpret
- Random Forest (RF): Less so
- **Desirable properties:**
 - Meaningful feature importance rather than rankings

Random Planted Forest (RPF): Additive Random Forest

Motivation



1

- Individual decision trees: Easy to interpret
- Random Forest (RF): Less so
- **Desirable properties:**
 - Meaningful feature importance rather than rankings
 - Quantification of main- **and interaction** effects

Random Planted Forest (RPF): Additive Random Forest

Motivation



1

- Individual decision trees: Easy to interpret
- Random Forest (RF): Less so
- **Desirable properties:**
 - Meaningful feature importance rather than rankings
 - Quantification of main- **and interaction** effects
- Additive models (LM, GAM, ...) can provide both

Random Planted Forest (RPF): Additive Random Forest

Motivation



1

- Individual decision trees: Easy to interpret
- Random Forest (RF): Less so
- **Desirable properties:**
 - Meaningful feature importance rather than rankings
 - Quantification of main- **and interaction** effects
- Additive models (LM, GAM, ...) can provide both
- → Need to manually specify interactions in model fit

Random Planted Forest (RPF): Additive Random Forest

Functional ANOVA Expansion



- Setting: Regression with target $Y_i \in \mathbb{R}^p$ and feature vector \mathbf{x}_i

Functional ANOVA Expansion



- Setting: Regression with target $Y_i \in \mathbb{R}^p$ and feature vector \mathbf{x}_i
- Decompose prediction $\mathbb{E}(Y_i|X = \mathbf{x}_i) = \hat{m}(\mathbf{x}_i)$ into

Functional ANOVA Expansion



- Setting: Regression with target $Y_i \in \mathbb{R}^p$ and feature vector \mathbf{x}_i
- Decompose prediction $\mathbb{E}(Y_i|X = \mathbf{x}_i) = \hat{m}(\mathbf{x}_i)$ into
 - Average prediction \hat{m}_0 (“intercept”)

Functional ANOVA Expansion



- Setting: Regression with target $Y_i \in \mathbb{R}^p$ and feature vector \mathbf{x}_i
- Decompose prediction $\mathbb{E}(Y_i|X = \mathbf{x}_i) = \hat{m}(\mathbf{x}_i)$ into
 - Average prediction \hat{m}_0 (“intercept”)
 - Terms \hat{m}_S with $S \subseteq \{1, \dots, s\}$

Functional ANOVA Expansion



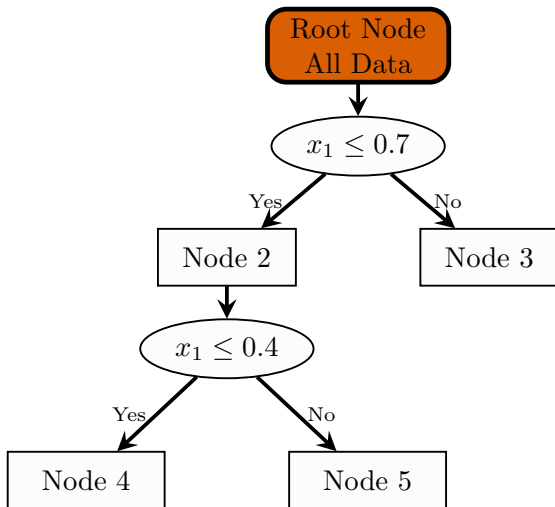
- Setting: Regression with target $Y_i \in \mathbb{R}^p$ and feature vector \mathbf{x}_i
- Decompose prediction $\mathbb{E}(Y_i|X = \mathbf{x}_i) = \hat{m}(\mathbf{x}_i)$ into
 - Average prediction \hat{m}_0 ("intercept")
 - Terms \hat{m}_S with $S \subseteq \{1, \dots, s\}$

Functional ANOVA Expansion

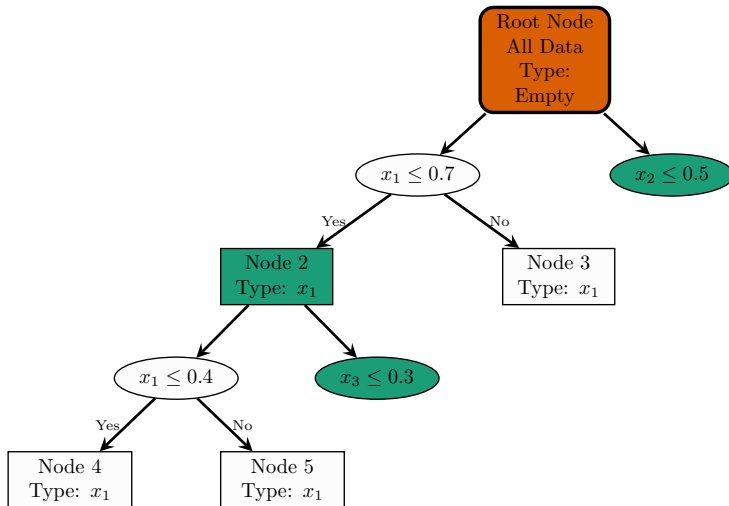
- Setting: Regression with target $Y_i \in \mathbb{R}^p$ and feature vector \mathbf{x}_i
- Decompose prediction $\mathbb{E}(Y_i|X = \mathbf{x}_i) = \hat{m}(\mathbf{x}_i)$ into
 - Average prediction \hat{m}_0 ("intercept")
 - Terms \hat{m}_S with $S \subseteq \{1, \dots, s\}$

$$\begin{aligned}
 \hat{m}(\mathbf{x}) = & \hat{m}_0 \\
 & + \underbrace{\hat{m}_1(x_1) + \hat{m}_2(x_2) + \hat{m}_3(x_3)}_{\text{Main effects}} \\
 & + \underbrace{\hat{m}_{1,2}(x_1, x_2) + \hat{m}_{1,3}(x_1, x_3) + \hat{m}_{2,3}(x_2, x_3)}_{\text{2nd order interactions}} \\
 & + \underbrace{\hat{m}_{1,2,3}(x_1, x_2, x_3)}_{\text{3rd order interaction}}
 \end{aligned}$$

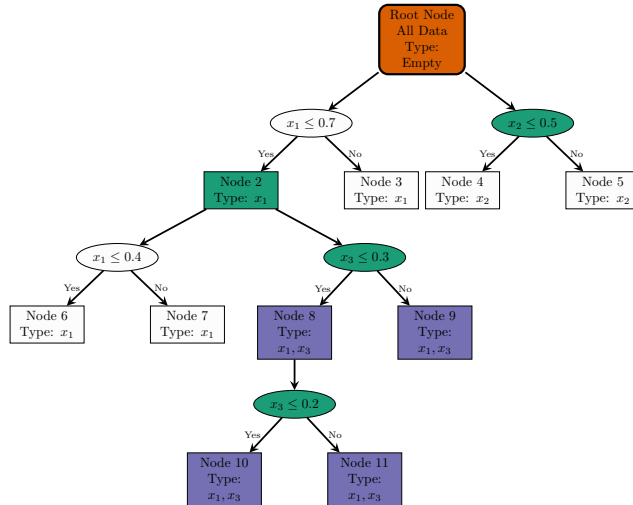
Trees in Random Forest



Planted Trees



Planted Trees



Key Differences of RPF to RF



6

- Splits some nodes multiple times (→ non-binary trees)

Key Differences of RPF to RF



6

- Splits some nodes multiple times (→ non-binary trees)
- Keeps track of features involved in split

Key Differences of RPF to RF



6

- Splits some nodes multiple times (→ non-binary trees)
- Keeps track of features involved in split
- Degree of interaction can be constrained

Key Differences of RPF to RF



6

- Splits some nodes multiple times (→ non-binary trees)
- Keeps track of features involved in split
- Degree of interaction can be constrained
- Stopping after adjustable number of splits

Key Differences of RPF to RF



6

- Splits some nodes multiple times (\rightarrow non-binary trees)
- Keeps track of features involved in split
- Degree of interaction can be constrained
- Stopping after adjustable number of splits
- Prediction is average of additive \hat{m}_S estimates

Application Example



7

- Bikeshare regression dataset ¹

¹from UCI ML repository

Application Example



7

- Bikeshare regression dataset ¹
- Target **bikers**: Number of bikers on a given day in 2011/2012

¹from UCI ML repository

Application Example



7

- Bikeshare regression dataset ¹
- Target **bikers**: Number of bikers on a given day in 2011/2012
- Focus on 3 features for example

¹from UCI ML repository

Application Example



7

- Bikeshare regression dataset ¹
- Target **bikers**: Number of bikers on a given day in 2011/2012
- Focus on 3 features for example
 - **hour** of day $\in \{0, 1, \dots, 23\}$

¹from UCI ML repository

Application Example



7

- Bikeshare regression dataset ¹
- Target **bikers**: Number of bikers on a given day in 2011/2012
- Focus on 3 features for example
 - **hour** of day $\in \{0, 1, \dots, 23\}$
 - **temp** normalized temperature $\in [0, 1]$

¹from UCI ML repository

Application Example



7

- Bikeshare regression dataset ¹
- Target **bikers**: Number of bikers on a given day in 2011/2012
- Focus on 3 features for example
 - **hour** of day $\in \{0, 1, \dots, 23\}$
 - **temp** normalized temperature $\in [0, 1]$
 - **workingday** binary $\rightarrow \{\text{workingday}, \text{no workingday}\}$

¹from UCI ML repository

Application Example



7

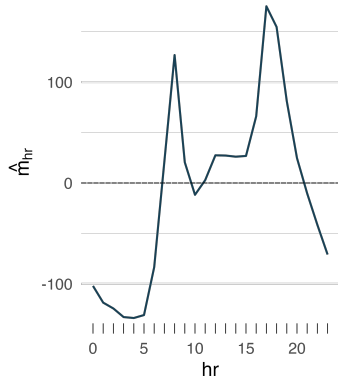
- Bikeshare regression dataset ¹
- Target **bikers**: Number of bikers on a given day in 2011/2012
- Focus on 3 features for example
 - **hour** of day $\in \{0, 1, \dots, 23\}$
 - **temp** normalized temperature $\in [0, 1]$
 - **workingday** binary $\rightarrow \{\text{workingday}, \text{no workingday}\}$
- Average prediction: $\hat{m}_0 \approx 143.7$

¹from UCI ML repository

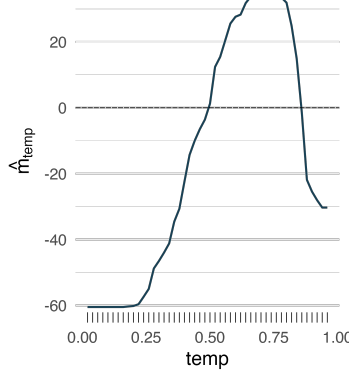
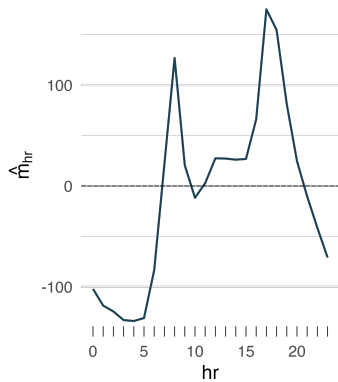
Main Effects



8



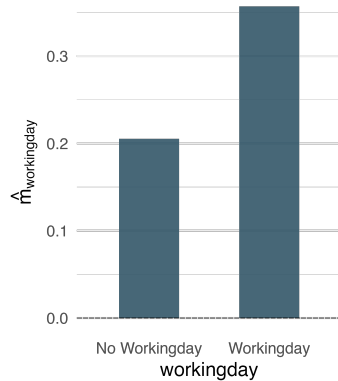
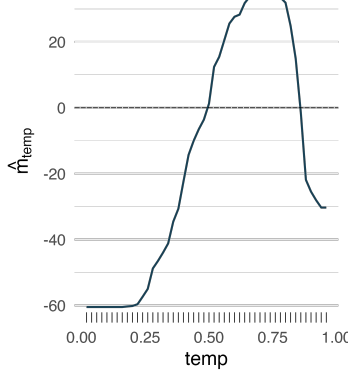
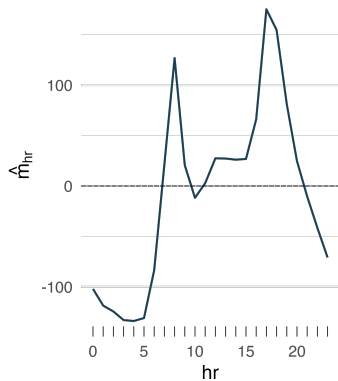
Main Effects



Main Effects



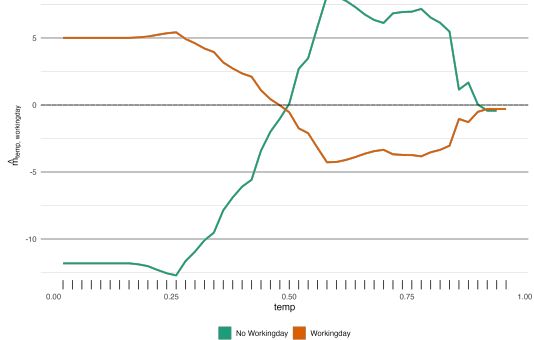
8



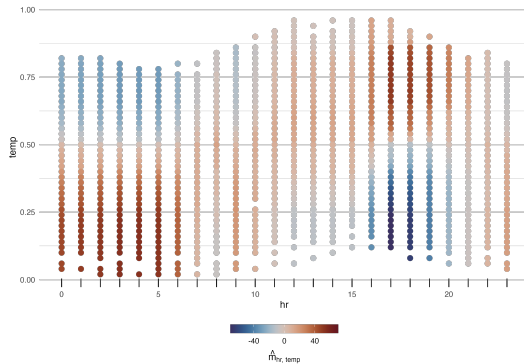
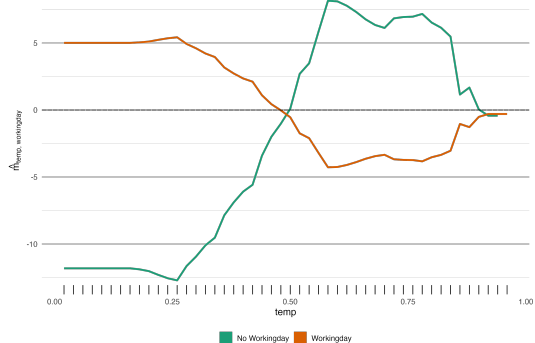
Hour \times Working Day: “Rush Hour Effect”



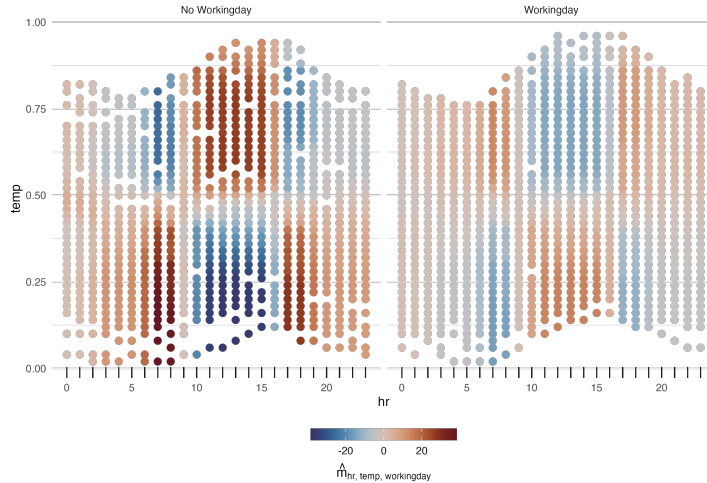
More 2nd Order Interactions



More 2nd Order Interactions



3rd Order Interaction



Feature Importance



12

- Average of absolute values of term of interest

Feature Importance



12

- Average of absolute values of term of interest

Feature Importance



12

- Average of absolute values of term of interest

$$\text{VI}_S(X) = \frac{1}{n} \sum_{i=1}^n |\hat{m}_S(\mathbf{x}_i)|$$

- Unlike RF Feature importance:

Feature Importance



12

- Average of absolute values of term of interest

$$\text{VI}_S(X) = \frac{1}{n} \sum_{i=1}^n |\hat{m}_S(\mathbf{x}_i)|$$

- Unlike RF Feature importance:
 - Scores [per interaction](#) term

Feature Importance



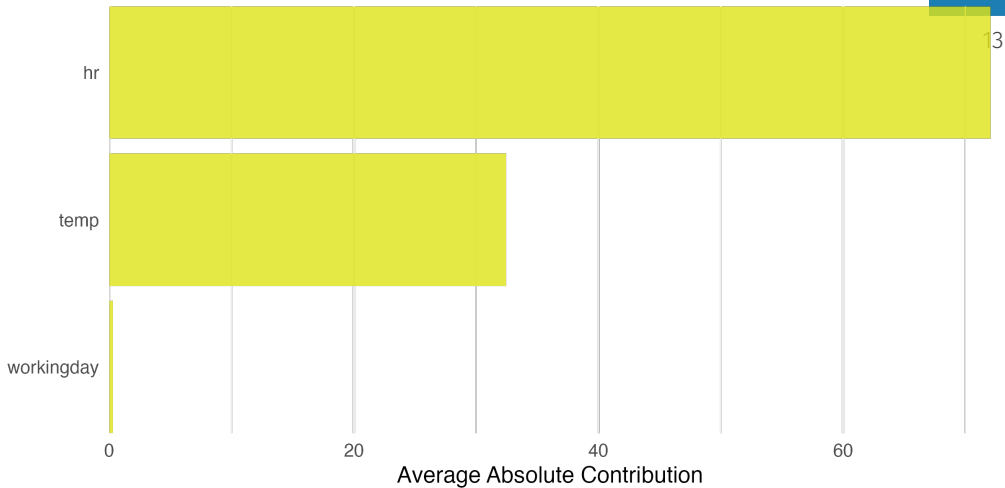
12

- Average of absolute values of term of interest

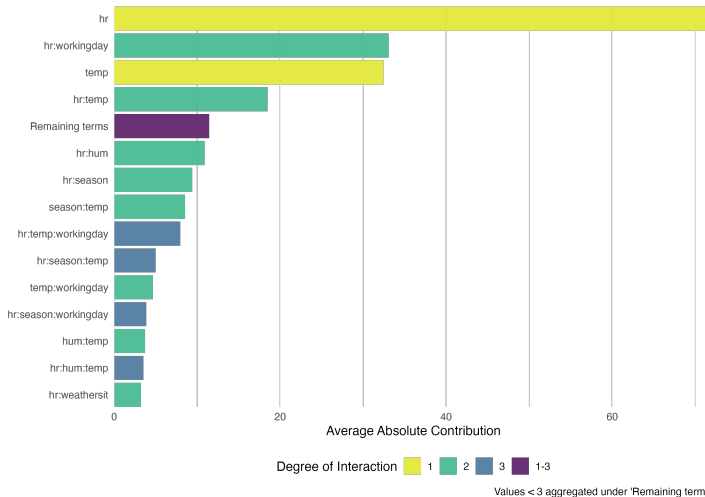
$$VI_S(X) = \frac{1}{n} \sum_{i=1}^n |\hat{m}_S(\mathbf{x}_i)|$$

- Unlike RF Feature importance:
 - Scores [per interaction](#) term
 - Importance scores on same scale as prediction

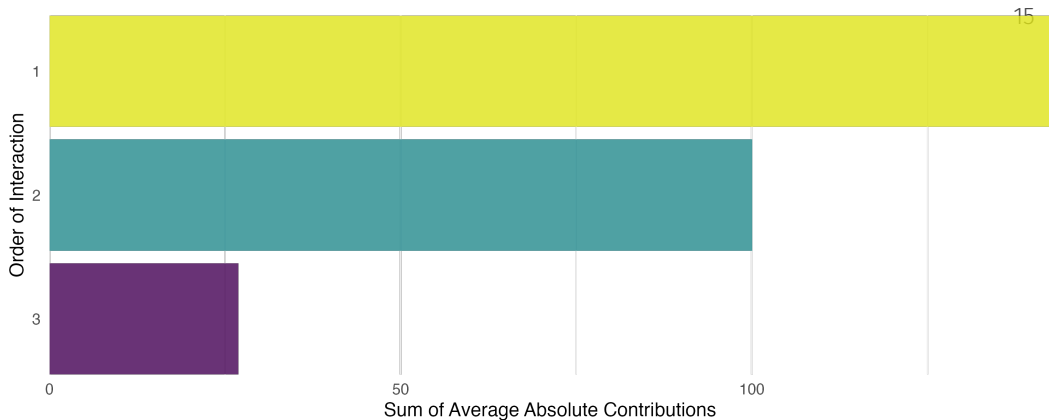
Feature Importance per Main Term



Feature Importance per All Terms



Feature Importance by Order of Interaction



Related work



16

Glex²: Same ANOVA decomposition but generally for tree-based methods (e.g. XGBoost)

- Idea:

²Hiabu, Meyer, and Wright (2023)

Related work



16

Glex²: Same ANOVA decomposition but generally for tree-based methods (e.g. XGBoost)

- Idea:
 - Fit XGBoost with more shallow trees (e.g. `max_depth = 4` \leftrightarrow `max_interaction = 4`)

²Hiabu, Meyer, and Wright (2023)

Related work



16

Glex²: Same ANOVA decomposition but generally for tree-based methods (e.g. XGBoost)

- Idea:

- Fit XGBoost with more shallow trees (e.g. `max_depth = 4` \leftrightarrow `max_interaction = 4`)
- Extract component-wise predictions from tree structure

²Hiabu, Meyer, and Wright (2023)

Related work



16

Glex²: Same ANOVA decomposition but generally for tree-based methods (e.g. XGBoost)

- **Idea:**
 - Fit XGBoost with more shallow trees (e.g. `max_depth = 4` \leftrightarrow `max_interaction = 4`)
 - Extract component-wise predictions from tree structure
- **Benefit:** Use existing / well known / well optimized algorithm

²Hiabu, Meyer, and Wright (2023)

Related work



16

Glex²: Same ANOVA decomposition but generally for tree-based methods (e.g. XGBoost)

- **Idea:**
 - Fit XGBoost with more shallow trees (e.g. `max_depth = 4` \leftrightarrow `max_interaction = 4`)
 - Extract component-wise predictions from tree structure
- **Benefit:** Use existing / well known / well optimized algorithm
- **Drawback:** Computationally intensive post-hoc computation

²Hiabu, Meyer, and Wright (2023)

No Free Lunch



17

Better interpretability → worse predictive performance?

No Free Lunch



17

Better interpretability → worse predictive performance?

- Benchmark comparing RPF with XGBoost, RF incl. tuning

No Free Lunch



17

Better interpretability → worse predictive performance?

- Benchmark comparing RPF with XGBoost, RF incl. tuning
- 28 datasets from OpenML-CTR23 regression benchmark suite ³

³Fischer et al. (2023)

No Free Lunch



17

Better interpretability → worse predictive performance?

- Benchmark comparing RPF with XGBoost, RF incl. tuning
- 28 datasets from OpenML-CTR23 regression benchmark suite ³
- Also comparing XGBoost / RPF with interactions restrained to 2

³Fischer et al. (2023)

No Free Lunch



17

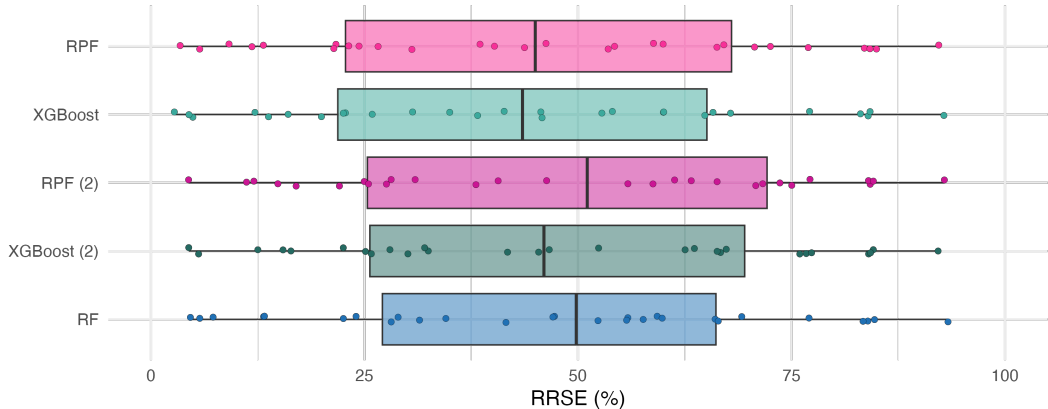
Better interpretability → worse predictive performance?

- Benchmark comparing RPF with XGBoost, RF incl. tuning
- 28 datasets from OpenML-CTR23 regression benchmark suite ³
- Also comparing XGBoost / RPF with interactions restrained to 2
- Generally XGBoost best, RPF and RF closely behind

³Fischer et al. (2023)

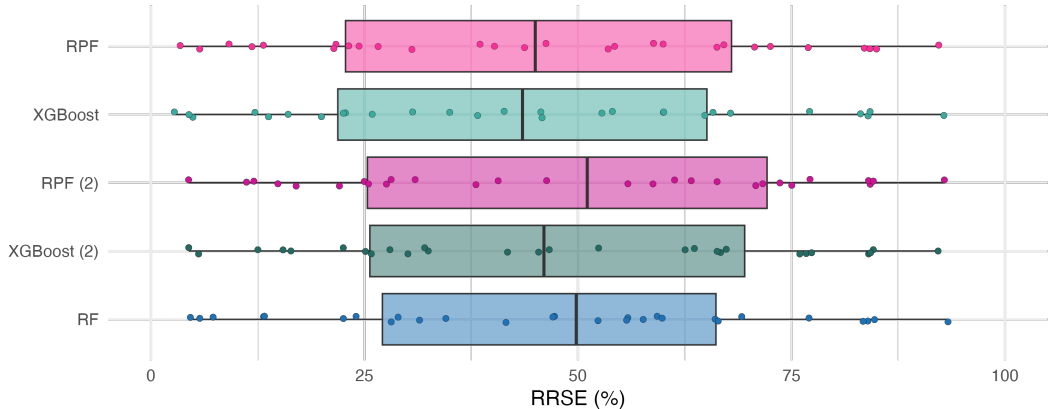
Benchmark Results (Aggregated)

- Root-Relative Squared Error (RRSE) $\sqrt{\frac{SSE(Y, \hat{Y})}{SSE(Y, \bar{Y})}}$

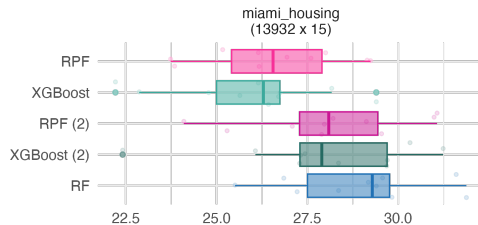
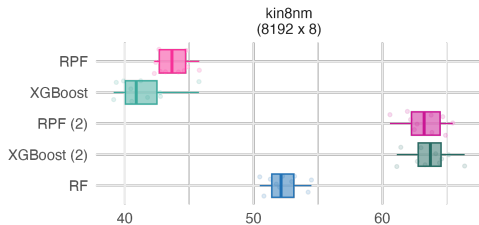
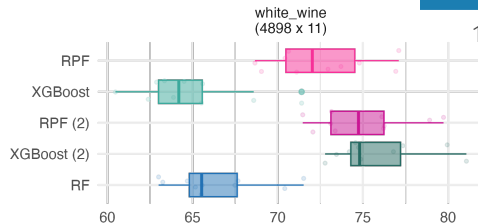
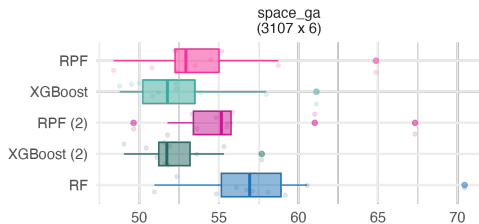


Benchmark Results (Aggregated)

- Root-Relative Squared Error (RRSE) $\sqrt{\frac{SSE(Y, \hat{Y})}{SSE(Y, \bar{Y})}}$
- Featureless model scores 1, perfect score 0



Results for Selected Tasks



RRSE (%)

Summary



20

Random Planted Forests = Additive Random Forests

- (+) Interpretability on global and local perspective

Summary



20

Random Planted Forests = Additive Random Forests

- (+) Interpretability on global and local perspective
- (+) Interpretable on same scale as target

Summary



20

Random Planted Forests = Additive Random Forests

- (+) Interpretability on global and local perspective
 - (+) Interpretable on same scale as target
 - (~) Predictive performance worse but similar to comparable algorithms
-

Summary



20

Random Planted Forests = Additive Random Forests

- (+) Interpretability on global and local perspective
 - (+) Interpretable on same scale as target
 - (~) Predictive performance worse but similar to comparable algorithms
 - (-) Computationally heavy for large data
-

Summary



20

Random Planted Forests = Additive Random Forests

- (+) Interpretability on global and local perspective
- (+) Interpretable on same scale as target
- (~) Predictive performance worse but similar to comparable algorithms
- (-) Computationally heavy for large data
- (+) R package available ⁴

⁴github.com/PlantedML/randomPlantedForest

Thank you for your attention!



Slides:

www.leibniz-bips.de/en

Contact

Lukas Burk

Leibniz Institute for Prevention Research
and Epidemiology – BIPS

Achterstraße 30
D-28359 Bremen



burk@leibniz-bips.de



References I



22

-  Fischer, Sebastian Felix et al. (2023). “OpenML-CTR23 – A Curated Tabular Regression Benchmarking Suite”. In: [AutoML Conference 2023 \(Workshop\)](#).
-  Hiabu, Munir, Joseph T. Meyer, and Marvin N. Wright (Apr. 11, 2023). “International Conference on Artificial Intelligence and Statistics”. In: [ISSN: 2640-3498 Citation Key: hiabu2023unifyinglocala](#). PMLR, pp. 7040–7060.