Random Planted Forest

A Directly Interpretable Tree Ensemble

Joseph T. Meyer[5] **Lukas Burk**[1,2,3,4] Munir Hiabu[6] Enno Mammen[5]

[1]Leibniz Institute for Prevention Research and Epidemiology – BIPS
[2]LMU Munich [3]University of Bremen
[4]Munich Center for Machine Learning (MCML)
[5]Heidelberg University [6]University of Copenhagen

DAGStat 2025 — March 27th, 2025

Motivation

- Tree-based methods like Random Forest (RF):

Motivation

- Tree-based methods like Random Forest (RF):
  - Fast & flexible

Motivation

- Tree-based methods like Random Forest (RF):
  - Fast & flexible
  - Interpretable? → It depends

Motivation

- Tree-based methods like Random Forest (RF):
  - Fast & flexible
  - Interpretable? → It depends
- Wishlist:

Motivation

- Tree-based methods like Random Forest (RF):
  - Fast & flexible
  - Interpretable? → It depends
- Wishlist:
  - Meaningful feature importance

Motivation

- Tree-based methods like Random Forest (RF):
  - Fast & flexible
  - Interpretable? → It depends
- Wishlist:
  - Meaningful feature importance
  - Quantification of main- and interaction effects

Motivation

- Tree-based methods like Random Forest (RF):
  - Fast & flexible
  - Interpretable? → It depends
- Wishlist:
  - Meaningful feature importance
  - Quantification of main- and interaction effects
- Additive models useful for both

Motivation

- Tree-based methods like Random Forest (RF):
  - Fast & flexible
  - Interpretable? → It depends
- Wishlist:
  - Meaningful feature importance
  - Quantification of main- and interaction effects
- Additive models useful for both

Motivation

- Tree-based methods like Random Forest (RF):
  - Fast & flexible
  - Interpretable? → It depends
- Wishlist:
  - Meaningful feature importance
  - Quantification of main- and interaction effects
- Additive models useful for both

→ **Random Planted Forest** (RPF): Additive Random Forest

Functional ANOVA Expansion

- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance $\mathbf{x}_i$

Functional ANOVA Expansion

- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance $\mathbf{x}_i$
- Expand prediction $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ into

Functional ANOVA Expansion

- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance $\mathbf{x}_i$
- Expand prediction $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ into
    - $\hat{m}_0$: Average prediction ("intercept") plus...

Functional ANOVA Expansion

- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance $\mathbf{x}_i$
- Expand prediction $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ into
  - $\hat{m}_0$: Average prediction ("intercept") plus...
  - Terms $\hat{m}_S$ with feature $S \subseteq \{1, \dots, p\}$

Functional ANOVA Expansion

- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance $\mathbf{x}_i$
- Expand prediction $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ into
  - $\hat{m}_0$: Average prediction ("intercept") plus...
  - Terms $\hat{m}_S$ with feature $S \subseteq \{1, \ldots, p\}$

Functional ANOVA Expansion

- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance $\mathbf{x}_i$
- Expand prediction $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ into
  - $\hat{m}_0$: Average prediction ("intercept") plus...
  - Terms $\hat{m}_S$ with feature $S \subseteq \{1, \dots, p\}$

$$
\begin{aligned}
\hat{m}(\mathbf{x}_i) = & \hat{m}_0 + \\
& \underbrace{\hat{m}_1(x_1) + \hat{m}_2(x_2) + \hat{m}_3(x_3)}_{\text{Main effect terms}} +
\end{aligned}
$$

Functional ANOVA Expansion

- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance $\mathbf{x}_i$
- Expand prediction $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ into
  - $\hat{m}_0$: Average prediction ("intercept") plus...
  - Terms $\hat{m}_S$ with feature $S \subseteq \{1, \ldots, p\}$

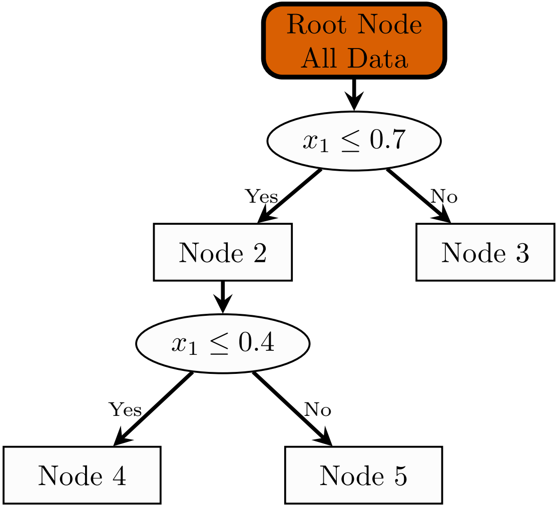
$$
\begin{aligned}
\hat{m}(\mathbf{x}_i) = & \hat{m}_0 + \\
& \underbrace{\hat{m}_1(x_1) + \hat{m}_2(x_2) + \hat{m}_3(x_3)}_{\text{Main effect terms}} + \\
& \underbrace{\hat{m}_{1,2}(x_1, x_2) + \hat{m}_{1,3}(x_1, x_3) + \hat{m}_{2,3}(x_2, x_3)}_{\text{2nd order interactions}} +
\end{aligned}
$$

Functional ANOVA Expansion

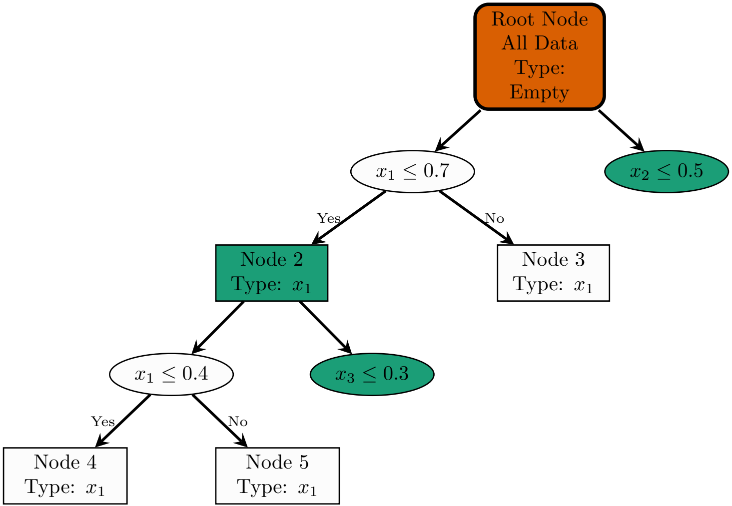
- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance $\mathbf{x}_i$
- Expand prediction $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ into
  - $\hat{m}_0$: Average prediction ("intercept")
  - Terms $\hat{m}_S$ with features $S \subseteq \{1, \dots, p\}$

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

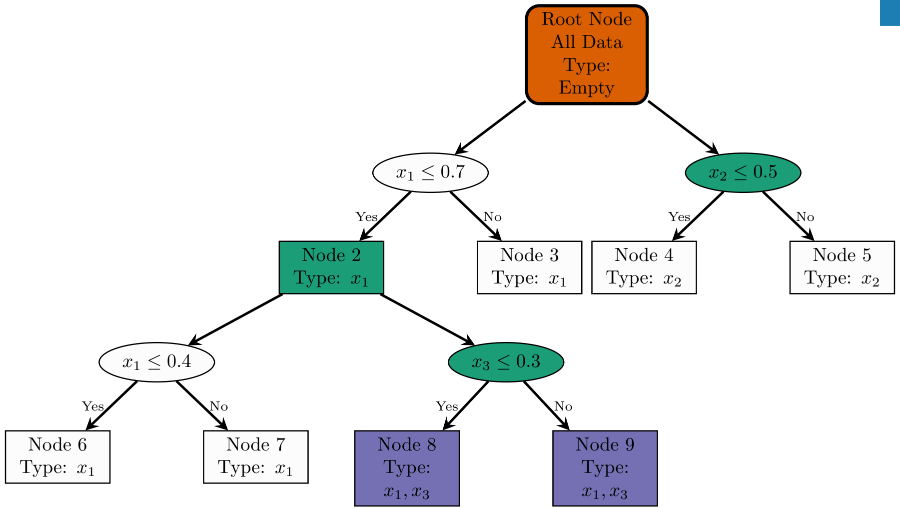
Trees in Random Forest



Planted Trees (I)



Planted Trees (II)



Key features of Random Planted Forests

- Ensemble of trees like RF

Key features of Random Planted Forests

- Ensemble of trees like RF
- Splits nodes multiple times (→ non-binary trees!)

Key features of Random Planted Forests

- Ensemble of trees like RF
- Splits nodes multiple times ($\rightarrow$ non-binary trees!)
- Nodes keep track of features involved in construction

Key features of Random Planted Forests

- Ensemble of trees like RF
- Splits nodes multiple times (→ non-binary trees!)
- Nodes keep track of features involved in construction
- Degree of interaction can be constrained

Key features of Random Planted Forests

- Ensemble of trees like RF
- Splits nodes multiple times ($\rightarrow$ non-binary trees!)
- Nodes keep track of features involved in construction
- Degree of interaction can be constrained
- Prediction built incrementally using residuals (cf. Gradient Boosting)

Key features of Random Planted Forests

- Ensemble of trees like RF
- Splits nodes multiple times (→ non-binary trees!)
- Nodes keep track of features involved in construction
- Degree of interaction can be constrained
- Prediction built incrementally using residuals (cf. Gradient Boosting)
- Tree stops after adjustable number of splits

Application Example

- `Bikeshare` regression dataset [1]

[1] from UCI ML repository

Application Example

- `Bikeshare` regression dataset [1]
- Target **`bikers`**: Number of bikers per hour in 2011/2012

[1] from UCI ML repository

Application Example

- `Bikeshare` regression dataset [1]
- Target **`bikers`**: Number of bikers per hour in 2011/2012
- Focus on 3 features for illustration

[1] from UCI ML repository

Application Example

- `Bikeshare` regression dataset [1]
- Target `bikers`: Number of bikers per hour in 2011/2012
- Focus on 3 features for illustration
  - `hour` of day $\in \{0, 1, \ldots, 23\}$

[1] from UCI ML repository

Application Example

- `Bikeshare` regression dataset [1]
- Target `bikers`: Number of bikers per hour in 2011/2012
- Focus on 3 features for illustration
  - `hour` of day $\in \{0, 1, \ldots, 23\}$
  - `temp` normalized temperature $\in [0, 1]$

[1] from UCI ML repository

Application Example

- `Bikeshare` regression dataset [1]
- Target `bikers`: Number of bikers per hour in 2011/2012
- Focus on 3 features for illustration
  - `hour` of day $\in \{0, 1, \ldots, 23\}$
  - `temp` normalized temperature $\in [0, 1]$
  - `workingday` $\in$ {`workingday`, `no workingday`}

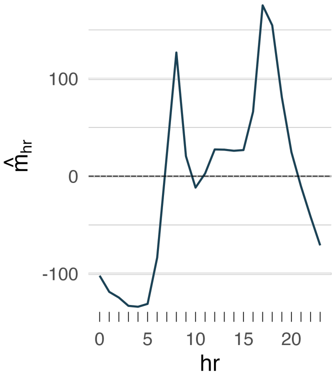
[1] from UCI ML repository

Application Example

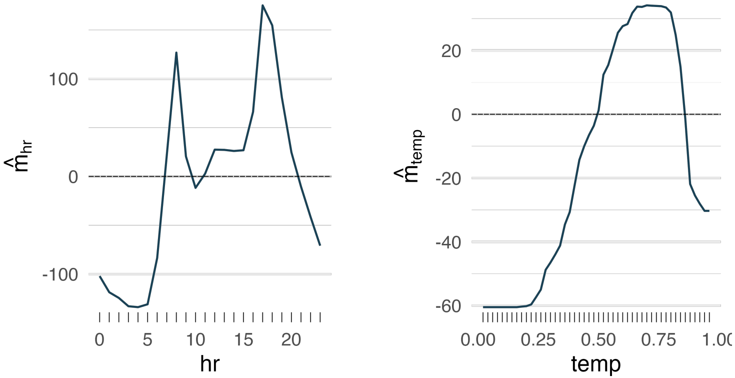
- `Bikeshare` regression dataset [1]
- Target **`bikers`**: Number of bikers per hour in 2011/2012
- Focus on 3 features for illustration
  - `hour` of day $\in \{0, 1, \dots, 23\}$
  - `temp` normalized temperature $\in [0, 1]$
  - `workingday` $\in$ {`workingday`, `no workingday`}
- Average prediction: $\hat{m}_0 \approx 144$

[1] from UCI ML repository

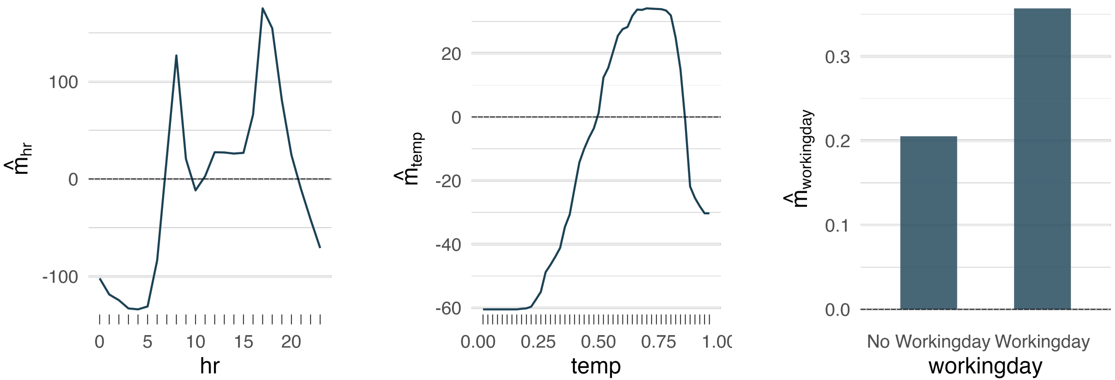
Main Effects



Main Effects

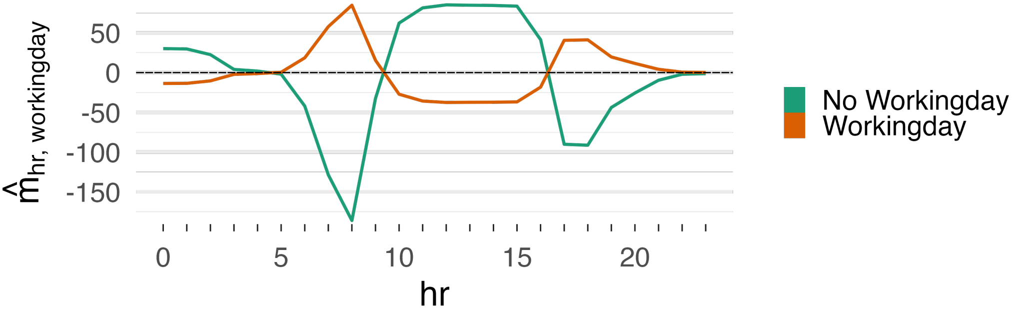


Main Effects



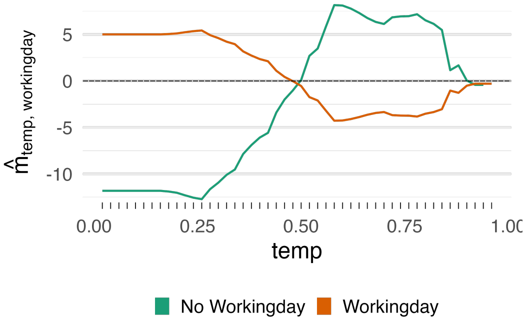
$$\hat{m} = \hat{m}_0 + \hat{m}_{\texttt{hr}}(\texttt{hr}) + \hat{m}_{\texttt{temp}}(\texttt{temp}) + \hat{m}_{\texttt{workingday}}(\texttt{workingday}) + \ldots$$

Hour × Working Day: "Rush Hour Effect"



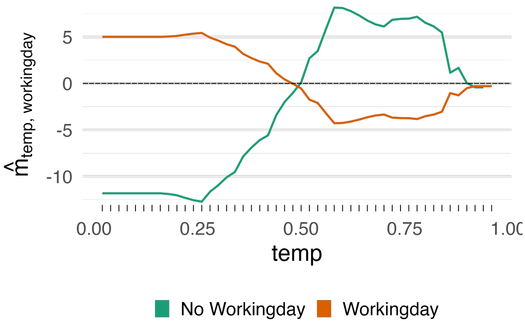
$$\ldots + \hat{m}_{\texttt{hr,workingday}}(\texttt{hr}, \texttt{workingday}) + \ldots$$

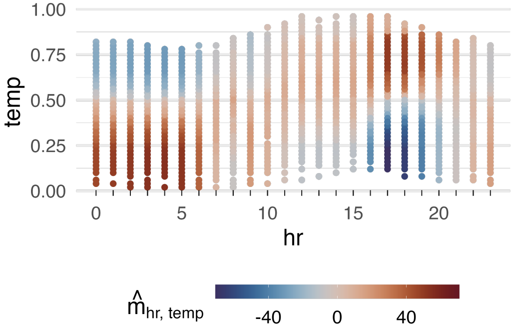
More 2nd Order Interactions



$$+\hat{m}_{\texttt{temp,workingday}}(\texttt{temp}, \texttt{workingday})$$

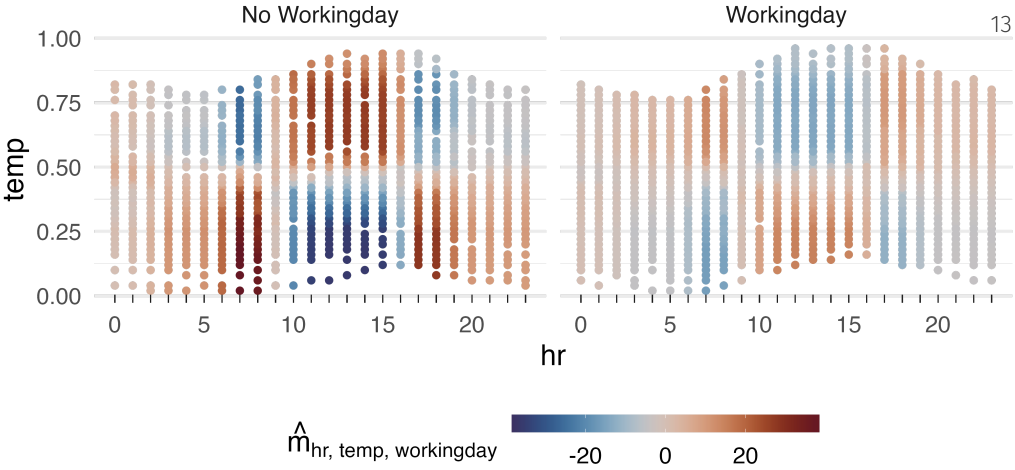
More 2nd Order Interactions





$$+\hat{m}_{\texttt{temp,workingday}}(\texttt{temp}, \texttt{workingday}) \qquad +\hat{m}_{\texttt{hr,temp}}(\texttt{hr}, \texttt{temp}) + \ldots$$

3rd Order Interaction



Feature Importance in RPF

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

- Average of absolute terms $\hat{m}_S$ for S of interest

Feature Importance in RPF

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

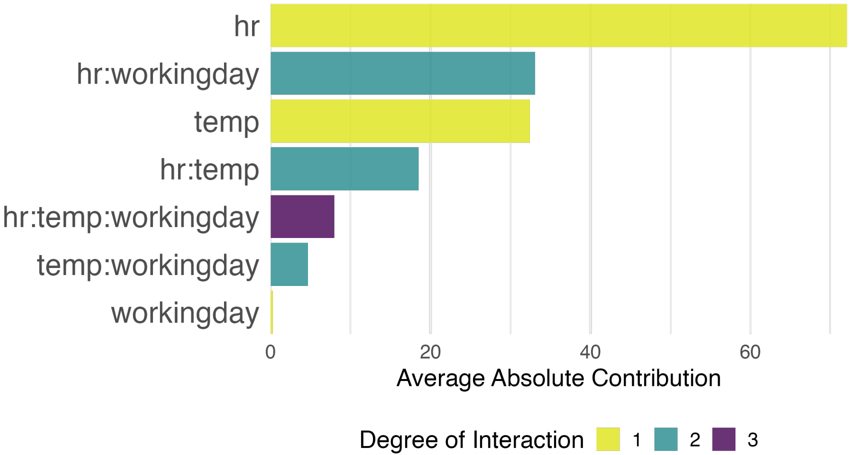
- Average of absolute terms $\hat{m}_S$ for S of interest
- Scores also per interaction term

Feature Importance in RPF

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

- Average of absolute terms $\hat{m}_S$ for S of interest
- Scores also per interaction term
- Importance scores on same scale as prediction

Feature Importance: All Terms



No Free Lunch

$(\uparrow)$ Gains in interpretability $\Rightarrow$ $(\downarrow)$ sacrifices in predictive performance?

No Free Lunch

$(\uparrow)$ Gains in interpretability $\Rightarrow$ $(\downarrow)$ sacrifices in predictive performance?

- Benchmark on **28** datasets [2] comparing RPF with XGBoost & RF

[2] OpenML-CTR23 regression benchmark suite: Fischer et al. (2023)

No Free Lunch

$(\uparrow)$ Gains in interpretability $\Rightarrow$ $(\downarrow)$ sacrifices in predictive performance?

- Benchmark on **28** datasets [2] comparing RPF with XGBoost & RF
- $\rightarrow$ RPF never best, rarely bad, usually close to XGBoost

[2] OpenML-CTR23 regression benchmark suite: Fischer et al. (2023)

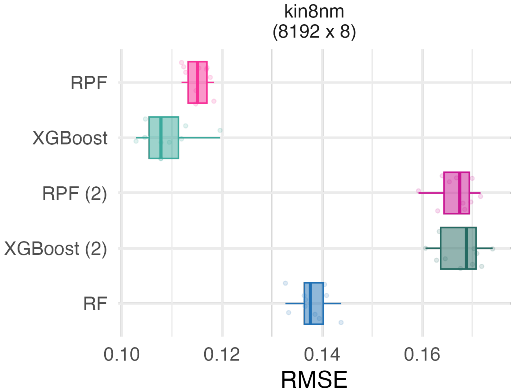
No Free Lunch

($\uparrow$) Gains in interpretability $\Rightarrow$ ($\downarrow$) sacrifices in predictive performance?

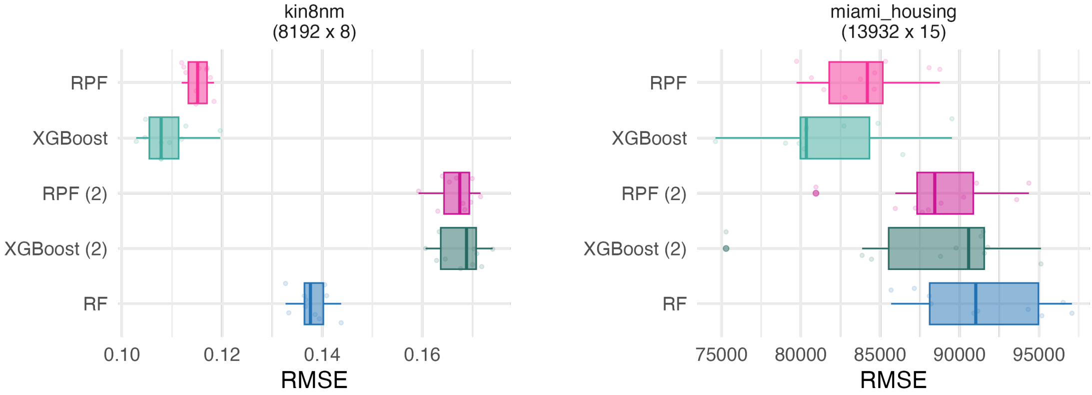
- Benchmark on **28** datasets [2] comparing RPF with XGBoost & RF
- $\rightarrow$ RPF never best, rarely bad, usually close to XGBoost
- RPF slower (especially with large data)

[2] OpenML-CTR23 regression benchmark suite: Fischer et al. (2023)

Benchmark Results (Selected Tasks)



Benchmark Results (Selected Tasks)



Summary

Random Planted Forests = Additive Random Forests

Summary

Random Planted Forests = Additive Random Forests

- ($\uparrow$) Feature importance on same scale as target

Summary

Random Planted Forests = Additive Random Forests

- ($\uparrow$) Feature importance on same scale as target
- ($\uparrow$) Main- and interaction effects

Summary

Random Planted Forests = Additive Random Forests

- ($\uparrow$) Feature importance on same scale as target
- ($\uparrow$) Main- and interaction effects
- ($\uparrow$) R package available [3]

[3] github.com/PlantedML/randomPlantedForest

Summary

Random Planted Forests = Additive Random Forests

- (↑) Feature importance on same scale as target
- (↑) Main- and interaction effects
- (↑) R package available [3]
- (→) Competetive predictive performance (mostly)

[3] github.com/PlantedML/randomPlantedForest

Summary

Random Planted Forests = Additive Random Forests

- ($\uparrow$) Feature importance on same scale as target
- ($\uparrow$) Main- and interaction effects
- ($\uparrow$) R package available [3]
- ($\rightarrow$) Competetive predictive performance (mostly)
- ($\downarrow$) Slower for large data (Optimization WIP!)

[3] github.com/PlantedML/randomPlantedForest

Thank you for your attention!

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

Fischer, Sebastian Felix et al. (2023). "OpenML-CTR23 – A Curated Tabular Regression Benchmarking Suite". In: AutoML Conference 2023 (Workshop).