

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



- 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
- Interpretability wishlist:

Motivation



- Tree-based methods like Random Forest (RF):
 - Fast & flexible
 - Interpretable? → It depends
- Interpretability wishlist:
 - Meaningful [feature importance](#)

Motivation



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

Motivation



1

- Tree-based methods like Random Forest (RF):
 - Fast & flexible
 - Interpretable? → It depends
- Interpretability wishlist:
 - Meaningful **feature importance**
 - Quantification of main- **and interaction effects**
- Additive models can provide both (with limitations)

Motivation



1

- Tree-based methods like Random Forest (RF):
 - Fast & flexible
 - Interpretable? → It depends
- Interpretability wishlist:
 - Meaningful **feature importance**
 - Quantification of main- **and interaction effects**
- Additive models can provide both (with limitations)

Motivation



1

- Tree-based methods like Random Forest (RF):
 - Fast & flexible
 - Interpretable? → It depends
- Interpretability wishlist:
 - Meaningful **feature importance**
 - Quantification of main- **and interaction effects**
- Additive models can provide both (with limitations)

→ **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 set $S \subseteq \{1, \dots, p\}$

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 set $S \subseteq \{1, \dots, p\}$

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 set $S \subseteq \{1, \dots, p\}$

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

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 set $S \subseteq \{1, \dots, p\}$

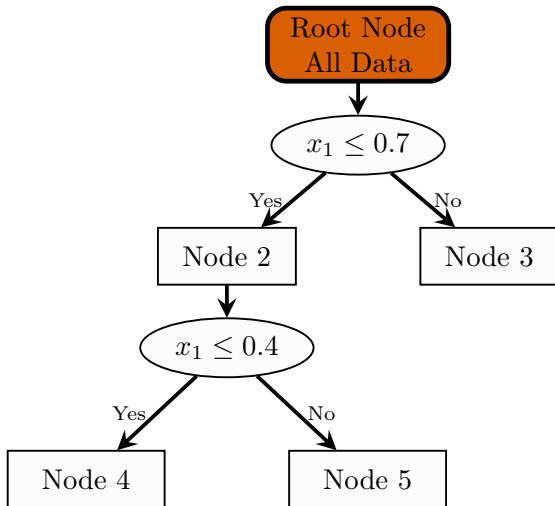
$$\begin{aligned}\hat{m}(\mathbf{x}_i) = & \hat{m}_0 + \\ & \underbrace{\hat{m}_1(x_1) + \hat{m}_2(x_2) + \hat{m}_3(x_3)}_{\text{Main effect terms}} + \\ & \underbrace{\hat{m}_{1,2}(x_1, x_2) + \hat{m}_{1,3}(x_1, x_3) + \hat{m}_{2,3}(x_2, x_3)}_{\text{2nd order interactions}} +\end{aligned}$$

Functional ANOVA Expansion

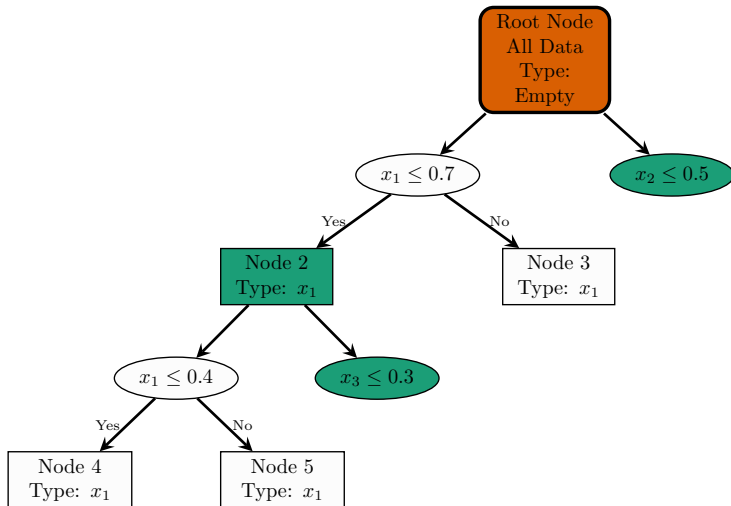
- Regression with target $Y_i \in \mathbb{R}$, features $X_i \in \mathbb{R}^p$, instance \mathbf{x}_i
- Expand prediction $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ into
 - \hat{m}_0 : Average prediction (“**intercept**”) plus...
 - Terms \hat{m}_S with feature set $S \subseteq \{1, \dots, p\}$

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

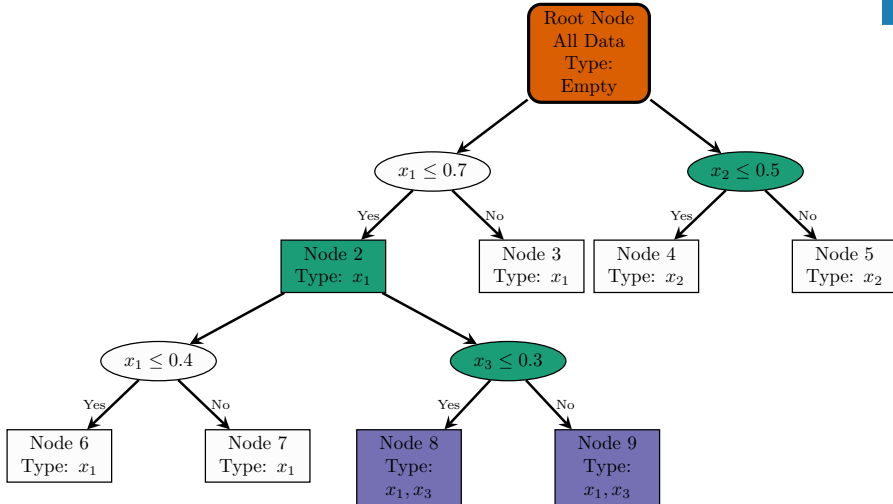
Trees in Random Forest



Planted Trees (I)



Planted Trees (II)



Key features of Random Planted Forests



8

- Ensemble of trees like RF

Key features of Random Planted Forests



8

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

Key features of Random Planted Forests



8

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

Key features of Random Planted Forests



8

- 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



8

- 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 up incrementally using residuals (cf. Gradient Boosting)

Key features of Random Planted Forests



8

- 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 up incrementally using residuals (cf. Gradient Boosting)
- Tree stops after adjustable **number of splits**

Application Example



9

- Bikeshare regression dataset ¹

¹from UCI ML repository

Application Example



9

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

¹from UCI ML repository

Application Example



9

- 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



9

- 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



9

- 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



9

- 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

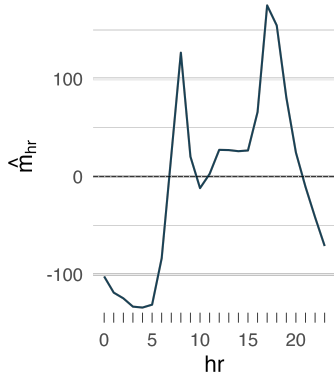


9

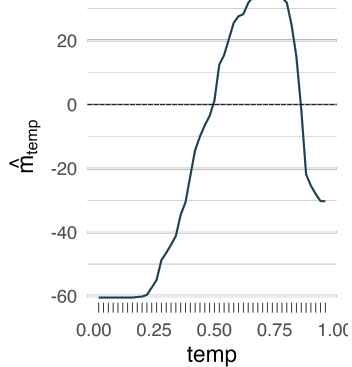
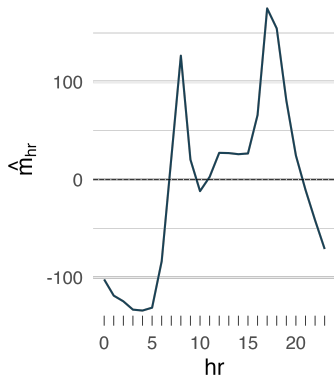
- Bikeshare regression dataset ¹
- Target **bikers**: Number of bikers on a given day in 2011/2012
- Focus on 3 features for example
 - **hour** of day $\in \{0, 1, \dots, 23\}$
 - **temp** normalized temperature $\in [0, 1]$
 - **workingday** binary $\rightarrow \{\text{workingday}, \text{no workingday}\}$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

¹from UCI ML repository

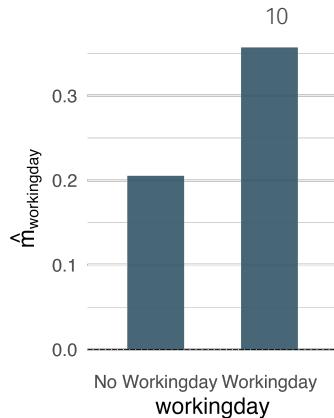
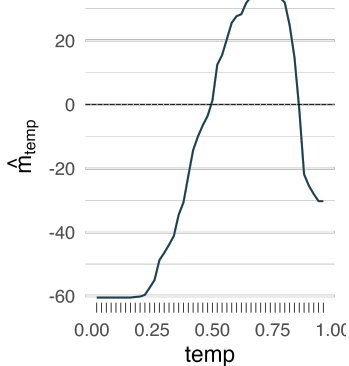
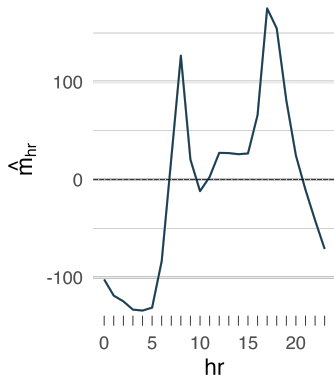
Main Effects



Main Effects

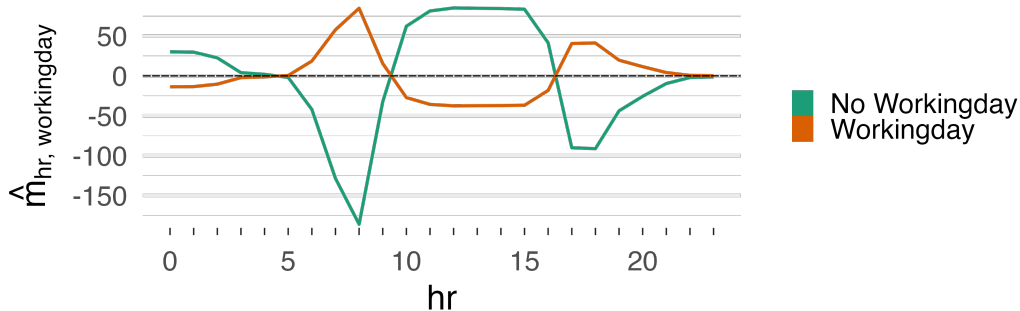


Main Effects



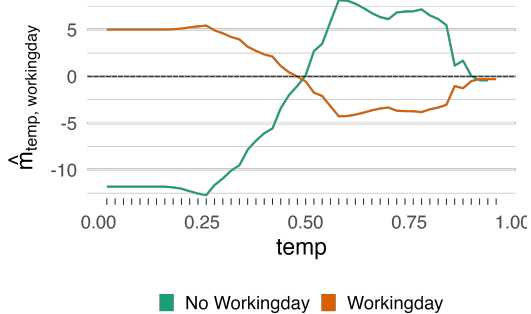
$$\hat{m} = \hat{m}_0 + \hat{m}_{hr}(hr) + \hat{m}_{temp}(temp) + \hat{m}_{workingday}(workingday) + \dots$$

Hour \times Working Day: “Rush Hour Effect”



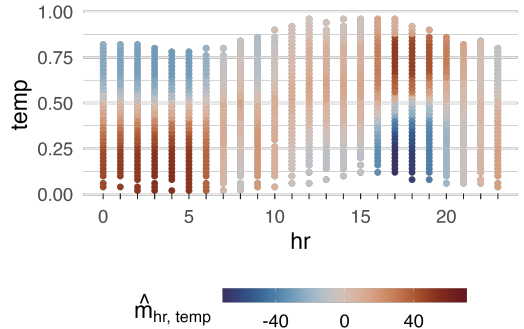
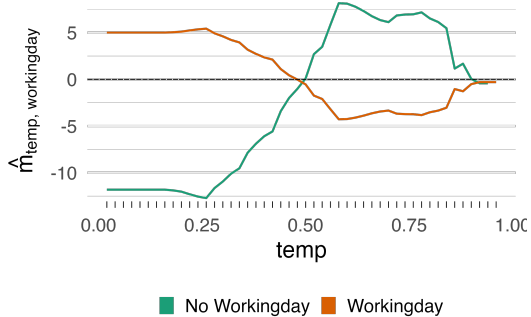
$$\dots + \hat{m}_{hr, workingday}(hr, workingday) + \dots$$

More 2nd Order Interactions



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

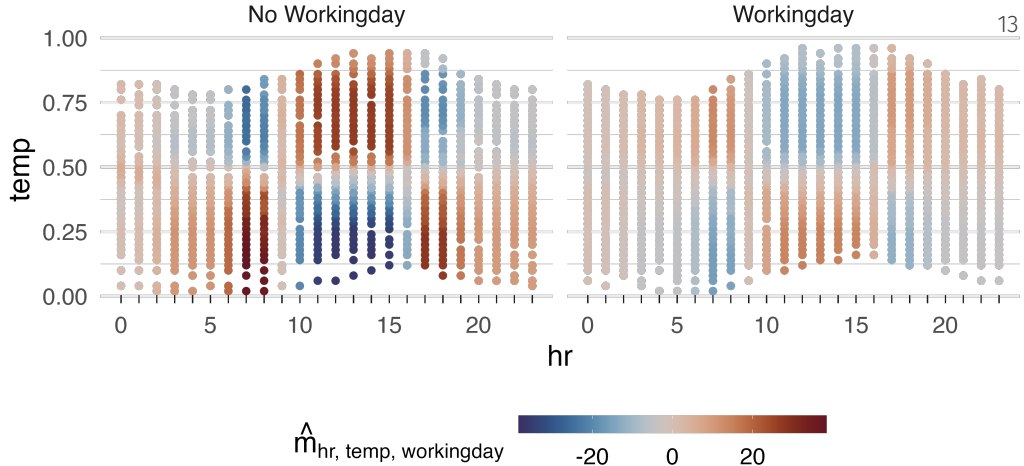
More 2nd Order Interactions



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

$$+\hat{m}_{hr, temp}(hr, temp) + \dots$$

3rd Order Interaction



Feature Importance in RPF



14

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

Feature Importance in RPF



14

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

Feature Importance in RPF



14

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

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

- Scores also [per interaction](#) term

Feature Importance in RPF



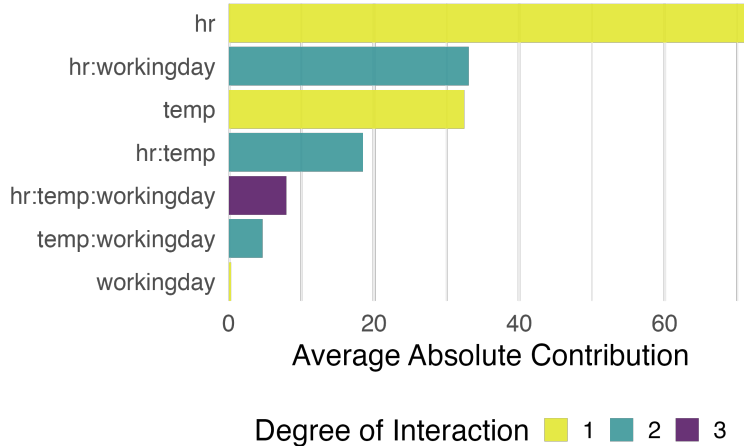
14

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

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

- Scores also **per interaction** term
- Importance scores on **same scale** as prediction

Feature Importance: All Terms



No Free Lunch



16

(↑) Gains in interpretability \Rightarrow (↓) sacrifices in predictive performance?

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

No Free Lunch



16

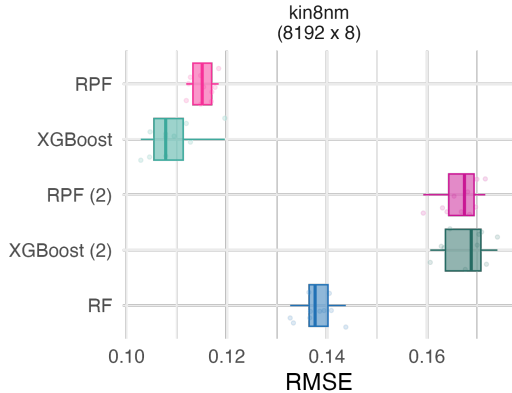
(↑) Gains in interpretability \Rightarrow (↓) sacrifices in predictive performance?

Benchmark on **28** datasets² comparing RPF with [XGBoost](#) & [RF](#)

→ RPF never best, rarely bad, usually close to XGBoost

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

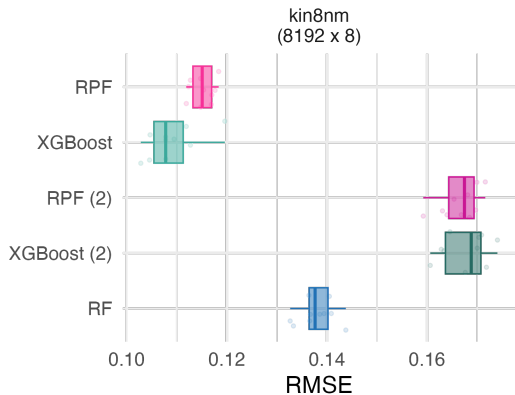
Benchmark Results (Selected Tasks)



Benchmark Results (Selected Tasks)



17



Summary



18

Random Planted Forests = Additive Random Forests

Summary



18

Random Planted Forests = Additive Random Forests

- (↑) Feature **importance** on same scale as target

Summary



18

Random Planted Forests = Additive Random Forests

- (↑) Feature **importance** on same scale as target
 - (↑) **Main-** and **interaction effects**
-

Summary



18

Random Planted Forests = Additive Random Forests

- (↑) Feature **importance** on same scale as target
- (↑) **Main-** and **interaction effects**
- (↑) R package available ³

³github.com/PlantedML/randomPlantedForest

Summary



18

Random Planted Forests = Additive Random Forests

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

³github.com/PlantedML/randomPlantedForest

Summary



18

Random Planted Forests = Additive Random Forests

- (↑) Feature **importance** on same scale as target
- (↑) **Main-** and **interaction effects**
- (↑) R package available ³
- (→) Competitive predictive performance (mostly)
- (↓) Slower for large data (Optimization WIP!)

³github.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



20

-  Fischer, Sebastian Felix et al. (2023). “OpenML-CTR23 – A Curated Tabular Regression Benchmarking Suite”. In: [AutoML Conference 2023 \(Workshop\)](#).