Diversity forests: Using split sampling to enable innovative complex split procedures in random forests

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Introduction

Diversity Forests

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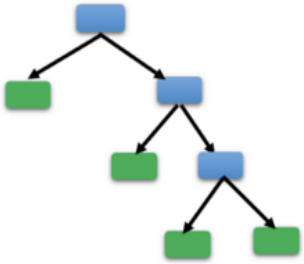
Conventional split finding vs. the diversity forest algorithm

Empirical results

Examples of complex split procedures



- Conventional **random forests** (RFs) feature **strong predictive** performance. ✓
- However, when considering **complex split procedures** (e.g., multivariable splitting) the **split finding scheme** used in the tree construction is (much) **too expensive** computationally. ✗
- But **complex split procedures** can **solve practically important problems** using random forests (e.g., detection of interaction effects). 😐
- The **diversity forest** (DF) **algorithm** (Hornung, 2022) is a new split finding scheme that **allows** for using **complex split procedures** in random forests. 🙂 ✓

Conventional split finding vs. the diversity forest algorithm

- Conventional **candidate split set** sampling:
  For $l = 1, \ldots,$ *mtry*:
  1. Randomly select one of the **covariates**.
  2. Evaluate **all** possible binary **splits** in the sampled covariate.
- The **DF algorithm** (slightly simplified):
  For $l = 1, \ldots,$ *nsplits*:
  1. Randomly select one so-called **split problem**.
  2. Randomly select and evaluate **one or few splits** in the sampled split problem.
- The **structures** of the **split problems** depend on the split procedure used;
  examples: univariable, binary splitting: all binary splits in a covariate x_j, multivariable splitting: all splits that involve one or several of the covariates x_{j_1}, x_{j_2}, and x_{j_3}

Empirical results (obtained for univariable, binary splitting)

- In a large-scale comparison study using 220 datasets it was seen that the **DF** algorithm is associated with a very **similar** (slightly better) **predictive performance** as conventional **RFs**.

- In an analysis using 50 datasets the **predictive performance** of DFs was seen to be quite **insensitive** to the choice of ***nsplits***.

  $\Rightarrow$ The value of ***nsplits*** does not have to be optimized, but using a **fixed value** is **sufficient**.

Interaction Forests – first published DF method with a complex split procedure

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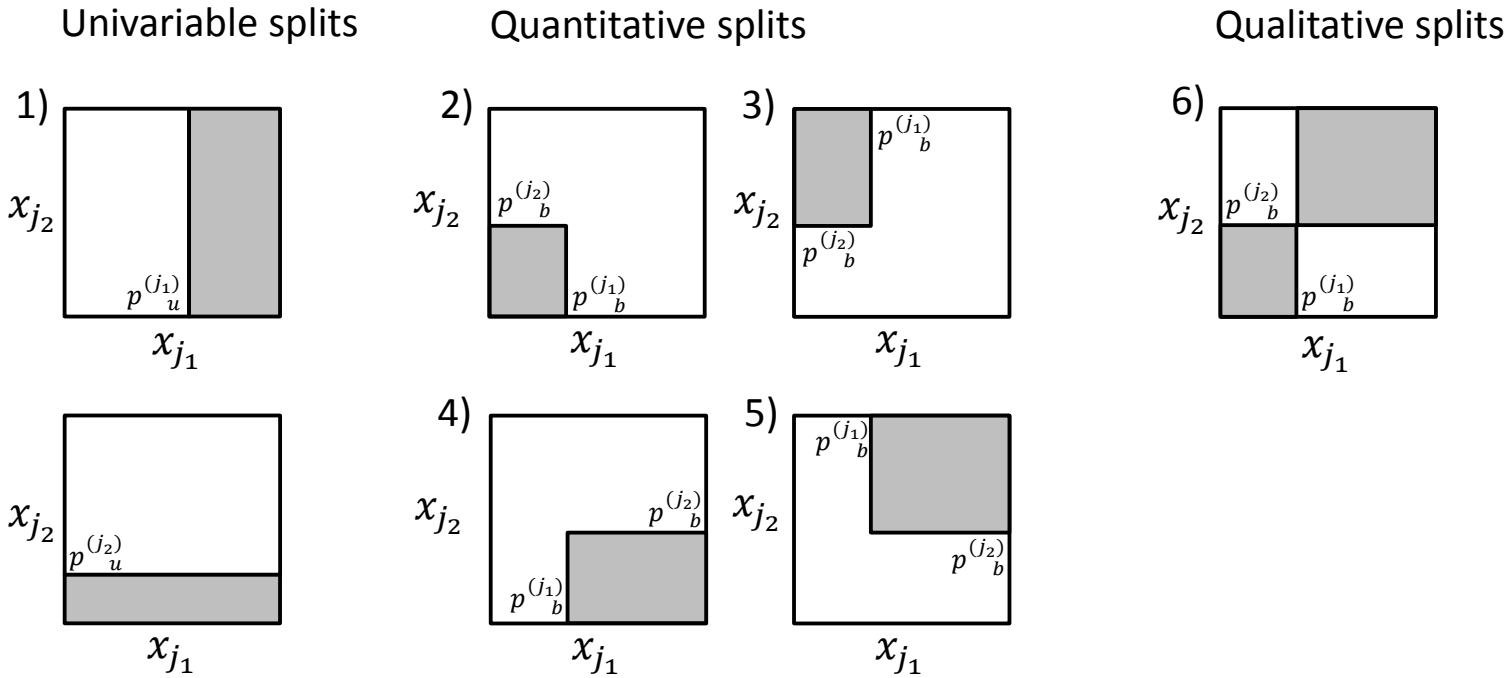
- Interaction Forests (Hornung & Boulesteix, 2022) use **bivariable splitting** to model **interaction effects** (R package `diversityForest`)
- **Ranking of interactions** with respect to their **importance to prediction** via the **E**ffect **I**mportance **M**easure



Outlook: Further potential complex split procedures

- **Multi-way splitting**: Tackling K**-class outcomes** with K-way splitting. $\Rightarrow$ **Better variable importance** measure values for **covariates that differentiate well between all** K **classes** instead of only a subset; more flexible splits for two-class, continuous, or survival outcomes

- **Detecting predictive patterns** by generating **diffuse** (bivariable) **partitions** of the covariate space

References – **Thank you for your attention!**

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