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# Distributional Regression Forests for Probabilistic Modeling and Forecasting 

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Motivation

## Motivation



LM, GLM
lm
glm

## Motivation



LM, GLM

lm<br>glm



GAM
mgcv
VGAM
...

## Motivation



LM, GLM

glm



GAM
mgcv
VGAM


## GAMLSS

gamlss mgcv VGAM
gamboostLSS

## Motivation



## Regression Tree


rpart
party (kit)

## Motivation



## Regression Tree

rpart
party (kit)



Random Forest

randomForest ranger
party(kit)

## Motivation



Regression Tree
Random Forest
Distributional trees and forests

| rpart | randomForest |
| :---: | :---: |
| party(kit) | ranger |
|  | party (kit) |

disttree based on partykit

## Goals

## Distributional:

- Specify the complete probability distribution (including location, scale, and shape).


## Tree:

- Automatic detection of steps and abrupt changes.
- Capture non-linear and non-additive effects and interactions.


## Forest:

- Smoother effects.
- Stabilization and regularization of the model.


## Distributional trees

DGP: $Y \mid X=x \sim \mathcal{N}\left(\mu(x), \sigma^{2}(x)\right)$


## Distributional trees



## Distributional trees



## Distributional trees



Distributional trees


## Global likelihood estimation

- Specify a parametric distribution family $F(\cdot ; \theta)$ with parameter vector $\theta \in \Theta$ capturing location, scale, shape.
- Cumulative distribution function and log-likelihood:

$$
\begin{aligned}
F(y ; \theta) & =\mathbb{P}_{\theta}(Y \leq y) \\
\ell(\theta ; y) & =\log (f(y ; \theta))
\end{aligned}
$$

- Estimate $\hat{\theta}$ via maximum likelihood based on a learning sample $y_{1}, \ldots, y_{n}$ :

$$
\hat{\theta}=\max _{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)
$$

## Adaptive local likelihood estimation

Idea: Covariates captured through adaptive weights.

$$
\hat{\theta}(\mathbf{x})=\max _{\theta \in \Theta} \sum_{i=1}^{n} w_{i}(\mathbf{x}) \cdot \ell\left(\theta ; y_{i}\right)
$$

Question: How to choose weighting function $w_{i}(\mathbf{x})$ ?
Possible answers: Based on learning sample $y_{1}, \ldots, y_{n}$ and (possibly new) observation $\mathbf{x}$.

- Tree: $w_{i}(\mathbf{x}) \in\{0,1\}$ indicates whether $\mathbf{x}$ and $y_{i}$ are classified into the same subgroup.
- Forest: $w_{i}(\mathbf{x}) \in[0,1]$ averages the weights for $\mathbf{x}$ and $y_{i}$ across trees.


## Distributional trees and forests

## Tree:

(1) Estimate $\hat{\theta}$ via maximum likelihood (without covariates).
(2) Test for associations or instabilities of the scores $\frac{\partial \ell}{\partial \theta}\left(\hat{\theta} ; y_{i}\right)$ and each partitioning variable $x_{i}$.
(3) Split the sample along the partitioning variable with the strongest association or instability. Choose breakpoint with highest improvement in log-likelihood.
(4) Repeat steps 1-3 recursively until some stopping criterion is met, yielding $B$ subgroups $\mathcal{B}_{b}$ with $b=1, \ldots, B$.

Forest: Ensemble of $T$ trees.

- Bootstrap or subsamples.
- Random input variable sampling.


## Adaptive local likelihood estimation

Estimator:

$$
\hat{\theta}(\mathbf{x})=\max _{\theta \in \Theta} \sum_{i=1}^{n} w_{i}(\mathbf{x}) \cdot \ell\left(\theta ; y_{i}\right)
$$

Weights:

$$
\begin{aligned}
w_{i}^{\text {base }}(\mathbf{x}) & =1 \\
w_{i}^{\text {tree }}(\mathbf{x}) & =\sum_{b=1}^{B} I\left(\left(\mathbf{x}_{i} \in \mathcal{B}_{b}\right) \wedge\left(\mathbf{x} \in \mathcal{B}_{b}\right)\right) \\
w_{i}^{\text {forest }}(\mathbf{x}) & =\frac{1}{T} \sum_{t=1}^{T} \sum_{b=1}^{B^{t}} I\left(\left(\mathbf{x}_{i} \in \mathcal{B}_{b}^{t}\right) \wedge\left(\mathbf{x} \in \mathcal{B}_{b}^{t}\right)\right)
\end{aligned}
$$

## Simulation

Models: disttree, distforest (100 trees), gamlss.

## Data:

$$
\begin{aligned}
y & \sim \mathcal{N}(\mu(x), \sigma(x)) \\
x & \sim \mathcal{U}(-0.4,1) \\
\mu(x) & =10 \cdot \exp \left\{-(4 \cdot x-2)^{2 \cdot \kappa}\right\} \\
\sigma(x) & =0.5+2 \cdot|x|
\end{aligned}
$$

## Parameters:

- 1 replication: $n=300, \kappa=2$.
- 150 replications: $n=1000, \kappa=1,8,15, \ldots, 71$.


## Simulation

True parameters


## Simulation

disttree


## Simulation

gamlss


## Simulation

distforest


## Simulation

disttree vs. distforest vs. gamlss


## Simulation

disttree vs. distforest vs. gamlss


## Simulation

disttree vs. distforest vs. gamlss


## Model specification

Covariates: Automatically through adaptive forest weights.
Response: Distributional specification needed.

- Continuous responses: Gaussian, ...
- Limited responses: Censored Gaussian, ...
- Survival times: Exponential, Weibull, ...
- Count: Poisson, negative binomial, ...

Guidance: Literature, theory, experience, ...
Alternative: Transformation models.

## Transformation models

## Advantages:

- Does not require specification of distribution family.
- More flexible framework.

Distribution function:

$$
F(y ; \theta)=\Phi\left(\mathbf{a}_{B s, d}(y)^{\top} \theta\right)
$$

- $\mathbf{a}_{B s, d}(y)^{\top} \theta$ is a smooth, monotone Bernstein polynomial of degree $d$.
- $d=1$ corresponds to $\mathcal{N}\left(\mu, \sigma^{2}\right)$.
- $d=5$ is surprisingly flexible.

Example: Body Mass Index explained by lifestyle factors
(Switzerland).

## Transformation models



## Software

Package: disttree available on R-Forge at https://R-Forge.R-project.org/projects/partykit/

## Main functions:

| distfit | Distributional fit (ML, gamlss.family/custom list). |
| :--- | :--- |
|  | No covariates. |
| disttree | Distributional tree (ctree/mob + distfit). <br>  <br> Covariates as partitioning variables. |
| distforest | Distributional forest (disttree ensemble). <br>  <br>  <br> Covariates as partitioning variables. |

## References

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