## $\square$ universität innsbruck

# Distributional Regression Forests for Probabilistic Modeling and Forecasting 

Achim Zeileis, Lisa Schlosser, Moritz N. Lang, Torsten Hothorn, Georg J. Mayr, Reto Stauffer
http://www.partykit.org/partykit/

Motivation

Motivation


LM, GLM

1m
glm

Motivation


LM, GLM


GAM
mgCV
VGAM

## Motivation



LM, GLM
lm
glm


GAM
mgcv
VGAM


GAMLSS
gamlss
mgcv
VGAM
gamboostLSS bamlss

## Motivation



Regression tree

rpart
party (kit)

## Motivation



Regression tree

rpart
party (kit)


Random forest

randomForest ranger party(kit)

## Motivation



## Motivation

## Distributional:

- Specify the complete probability distribution (location, scale, 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

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



## Distributional trees

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



## Distributional trees

Model: disttree (y ~ x)


## Distributional trees

Model: disttree (y ~ x)


## Distributional trees

Model: disttree (y ~ x)


Learning distributional trees and forests

## Tree:

Learning distributional trees and forests

## Tree:

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood
$\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood
$\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood

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

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ : Estimate $\hat{\theta}$ via maximum likelihood $\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$


## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood
$\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$
(2) Test for associations/instabilities of the scores


## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood $\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$
(2) Test for associations/instabilities of the scores
 $\frac{\partial \ell}{\partial \theta}\left(\hat{\theta} ; y_{i}\right)$ and each covariate $X_{i}$.
(3) Split along the covariate $X$ with strongest association or instability and at breakpoint $p$ with highest improvement in log-likelihood.

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood $\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$
(2) Test for associations/instabilities of the scores
 $\frac{\partial \ell}{\partial \theta}\left(\hat{\theta} ; y_{i}\right)$ and each covariate $X_{i}$.
(3) Split along the covariate $X$ with strongest association or instability and at breakpoint $p$ with highest improvement in log-likelihood.

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood $\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$
(2) Test for associations/instabilities of the scores
 $\frac{\partial \ell}{\partial \theta}\left(\hat{\theta} ; y_{i}\right)$ and each covariate $X_{i}$.
(3) Split along the covariate $X$ with strongest association or instability and at breakpoint $p$ 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 $b=1, \ldots, B$.

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood $\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$
(2) Test for associations/instabilities of the scores
 $\frac{\partial \ell}{\partial \theta}\left(\hat{\theta} ; y_{i}\right)$ and each covariate $X_{i}$.
(3) Split along the covariate $X$ with strongest association or instability and at breakpoint $p$ 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 $b=1, \ldots, B$.

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ :

Estimate $\hat{\theta}$ via maximum likelihood $\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$
(2) Test for associations/instabilities of the scores $\frac{\partial \ell}{\partial \theta}\left(\hat{\theta} ; y_{i}\right)$ and each covariate $X_{i}$.

(3) Split along the covariate $X$ with strongest association or instability and at breakpoint $p$ 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 $b=1, \ldots, B$.

## Learning distributional trees and forests

## Tree:

(1) Fit global distributional model $\mathcal{D}(Y ; \theta)$ : Estimate $\hat{\theta}$ via maximum likelihood $\hat{\theta}=\operatorname{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \ell\left(\theta ; y_{i}\right)$
(2) Test for associations/instabilities of the scores $\frac{\partial \ell}{\partial \theta}\left(\hat{\theta} ; y_{i}\right)$ and each covariate $X_{i}$.

(3) Split along the covariate $X$ with strongest association or instability and at breakpoint $p$ 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

## Parameter estimator for a global

 model with learning data $\left\{y_{i}\right\}_{i=1, \ldots, n}$ :$$
\hat{\theta} \quad=\underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{i=1}^{n} \quad \ell\left(\theta ; y_{i}\right)
$$

## Adaptive local likelihood estimation

## Parameter estimator for a global

 model with learning data $\left\{\left(y_{i}, \mathbf{x}_{i}\right)\right\}_{i=1, \ldots, n}$ :$$
\hat{\theta}(\mathbf{x})=\underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{i=1}^{n} w_{i}(\mathbf{x}) \cdot \ell\left(\theta ; y_{i}\right)
$$

## Adaptive local likelihood estimation

## Parameter estimator for a global

 model with learning data $\left\{\left(y_{i}, \mathbf{x}_{i}\right)\right\}_{i=1, \ldots, n}$ :$$
\hat{\theta}(\mathbf{x})=\underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{i=1}^{n} w_{i}(\mathbf{x}) \cdot \ell\left(\theta ; y_{i}\right)
$$

## Weights:

$$
w_{i}^{\text {base }}(\mathbf{x})=1
$$

## Adaptive local likelihood estimation

## Parameter estimator for an adaptive local

 model with learning data $\left\{\left(y_{i}, \mathbf{x}_{i}\right)\right\}_{i=1, \ldots, n}$ :$$
\hat{\theta}(\mathbf{x})=\underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{i=1}^{n} w_{i}(\mathbf{x}) \cdot \ell\left(\theta ; y_{i}\right)
$$

## Weights:

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

## Adaptive local likelihood estimation

## Parameter estimator for an adaptive local

 model with learning data $\left\{\left(y_{i}, \mathbf{x}_{i}\right)\right\}_{i=1, \ldots, n}$ :$$
\hat{\theta}(\mathbf{x})=\underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{i=1}^{n} w_{i}(\mathbf{x}) \cdot \ell\left(\theta ; y_{i}\right)
$$

## Weights:

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

## Weather forecasting

## Goal:



## Data:

- X: State of the atmosphere now (temperature, precipitation, wind, ...).
- Y: State of the atmosphere in the future (hours, days, weeks, ...).


## Weather forecasting

## Goal:



## Data:

- X: State of the atmosphere now (temperature, precipitation, wind, ...).
- Y: State of the atmosphere in the future (hours, days, weeks, ... ).


## Weather forecasting

## Goal:



## Two stages:

- Physical model: Numerical weather prediction (NWP).
- Statistical model: Model output statistics (MOS).


## Weather forecasting

## NWP:

- Based on a physical model.
- Massive numerical simulation of atmospheric processes.
- Here: Global model on a $50 \times 50 \mathrm{~km}^{2}$ grid.

Problem: Uncertain initial conditions, unresolved processes.
Solution: Ensemble of simulation runs under perturbed conditions.

## Weather forecasting

Global Forecast System (GFS) Ensemble Forecast for Innsbruck, Airport Forecast initialized 2018-03-13 00:00 UTC


## Weather forecasting

Global Forecast System (GFS) Ensemble Forecast for Innsbruck, Airport Forecast initialized 2018-03-13 00:00 UTC


## Weather forecasting

Global Forecast System (GFS) Ensemble Forecast for Innsbruck, Airport Forecast initialized 2018-03-13 00:00 UTC


## Weather forecasting

Global Forecast System (GFS) Ensemble Forecast for Innsbruck, Airport Forecast initialized 2018-03-13 00:00 UTC


## Weather forecasting

Global Forecast System (GFS) Ensemble Forecast for Innsbruck, Airport Forecast initialized 2018-03-13 00:00 UTC

$\begin{array}{lllllllll}\text { Mar } 14 & \text { Mar 15 } & \text { Mar 16 } & \text { Mar 17 } & \text { Mar 18 } & \text { Mar } 19 & \text { Mar 20 } & \text { Mar 21 } & \text { Mar } 22\end{array}$

## Precipitation forecasting

Goal: Predict daily precipitation amount in complex terrain.

## Precipitation forecasting

Goal: Predict daily precipitation amount in complex terrain.
Observation data: National Hydrographical Service.

- Daily 24 h precipitation sums from July over 28 years (1985-2012).
- 95 observation stations in Tyrol, Austria.


## Precipitation forecasting

Goal: Predict daily precipitation amount in complex terrain.
Observation data: National Hydrographical Service.

- Daily 24 h precipitation sums from July over 28 years (1985-2012).
- 95 observation stations in Tyrol, Austria.

NWP: Global Ensemble Forecast System.

- Model outputs: Precipitation, temperature, air pressure, convective available potential energy, downwards short wave radiation flux, ...
- 80 covariates based on ensemble min/max/mean/standard deviation.


## Precipitation forecasting

Goal: Predict daily precipitation amount in complex terrain.
Observation data: National Hydrographical Service.

- Daily 24 h precipitation sums from July over 28 years (1985-2012).
- 95 observation stations in Tyrol, Austria.

NWP: Global Ensemble Forecast System.

- Model outputs: Precipitation, temperature, air pressure, convective available potential energy, downwards short wave radiation flux, ...
- 80 covariates based on ensemble min/max/mean/standard deviation.

Distribution assumption: Power-transformed Gaussian, censored at 0.

$$
(\text { precipitation })^{\frac{1}{1.6}} \sim \mathcal{N}\left(\mu, \sigma^{2}\right)
$$

## Precipitation forecasting

Application for one station: Axams.

- Learn forest model on data from 24 years (1985-2008).
- Evaluate on 4 years (2009-2012). Here: July 24.



## Precipitation forecasting

Application for one station: Axams.

- Learn forest model on data from 24 years.
- Evaluate on 4 years.
- 10 times 7 -fold cross validation.

Benchmark: Against other heteroscedastic censored Gaussian models.

- Ensemble MOS: Linear predictors using only total precipitation.
- Prespecified GAMLSS: Variable selection based on expert knowledge.
- Boosted GAMLSS: Automatic variable selection.

Evaluation: Continuous ranked probability skill score.

## Precipitation forecasting

Cross validation (with reference model EMOS)


## Precipitation forecasting

## Application for all 95 stations:

- Learn forest model on data from 24 years (1985-2008).
- Evaluate on 4 years (2009-2012).
- Benchmark against other heteroscedastic censored Gaussian models.


## Precipitation forecasting

## Stations in Tyrol



## Wind forecasting

Goal: Nowcasting (1-3 hours ahead) of wind direction at Innsbruck Airport.

## Wind forecasting

Goal: Nowcasting (1-3 hours ahead) of wind direction at Innsbruck Airport.
Challenges:

- Circular response in $\left[0^{\circ}, 360^{\circ}\right)$ with $0^{\circ}=360^{\circ}$.
- Possibly abrupt changes due to geographical position.
- NWP outputs are less useful due to short lead time.


## Wind forecasting

Goal: Nowcasting (1-3 hours ahead) of wind direction at Innsbruck Airport.

## Challenges:

- Circular response in $\left[0^{\circ}, 360^{\circ}\right)$ with $0^{\circ}=360^{\circ}$.
- Possibly abrupt changes due to geographical position.
- NWP outputs are less useful due to short lead time.

Inputs: Observation data only (41,979 data points).

- 4 stations at Innsbruck Airport, 6 nearby weather stations.
- Base variables: Wind direction, wind (gust) speed, temperature, (reduced) air pressure, relative humidity.
- 260 covariates based on means/minima/maxima, temporal changes, spatial differences towards the airport.


## Wind forecasting



## Wind forecasting

Distribution assumption: Von Mises.

- Circular normal distribution.
- Location parameter $\mu \in[0,2 \pi)$.
- Concentration parameter $\kappa>0$.


Log-likelihood: $y \in[0,2 \pi)$ and parameter vector $\theta=(\mu, \kappa)$.

$$
\ell(\theta ; y)=\log \left\{\frac{1}{2 \pi I_{0}(\kappa)} e^{\kappa \cos (y-\mu)}\right\}
$$

where $I_{0}(\kappa)$ is the modified Bessel function of the first kind and order 0.

## Wind forecasting

Distribution assumption: Von Mises.

- Circular normal distribution.
- Location parameter $\mu \in[0,2 \pi)$.
- Concentration parameter $\kappa>0$.


Log-likelihood: $y \in[0,2 \pi)$ and parameter vector $\theta=(\mu, \kappa)$.

$$
\ell(\theta ; y)=\log \left\{\frac{1}{2 \pi I_{0}(\kappa)} e^{\kappa \cos (y-\mu)}\right\}
$$

where $I_{0}(\kappa)$ is the modified Bessel function of the first kind and order 0 .

## Wind forecasting



## Wind forecasting

Benchmark: Against other naive and circular models.

- Climatology: Without covariates.
- Persistency: Based on current wind direction.
- Circular GLM: Based on current wind speed and wind vectors (u,v).


## Wind forecasting

Evaluation: CRPS skill score for 1-hourly predictions (5-fold cross validation).


## Wind forecasting

Evaluation: CRPS skill score for 3-hourly predictions (5-fold cross validation).


## Transformation models

Alternative: When no obvious classic distribution assumption is available.

## 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

Software: disttree and circtree available on R-Forge at
https://R-Forge.R-project.org/projects/partykit/

## Main functions:

| distfit | Distributional fits (ML, gamlss.family/custom list). |
| :--- | :--- |
|  | No covariates. |
| disttree | Distributional trees (ctree/mob + distfit). <br> Covariates as partitioning variables. |
| distforest | Distributional forests (ensemble of disttrees). <br>  Covariates as partitioning variables. |

Correspondingly: circtree, circforest

## References

Schlosser L, Hothorn T, Stauffer R, Zeileis A (2019). "Distributional Regression Forests for Probabilistic Precipitation Forecasting in Complex Terrain." The Annals of Applied Statistics, 13(3), 1564-1589. doi:10.1214/19-A0AS1247

Schlosser L, Lang MN, Hothorn T, Mayr GJ, Stauffer R, Zeileis A (2019). "Distributional Trees for Circular Data." Proceedings of the 34th International Workshop on Statistical Modelling, 1, 226-231. https://eeecon.uibk.ac.at/~zeileis/papers/Schlosser+Lang+Hothorn-2019.pdf

Hothorn T, Zeileis A (2017). "Transformation Forests." arXiv 1701.02110, arXiv.org E-Print Archive. http://arxiv.org/abs/1701. 02110

Hothorn T, Hornik K, Zeileis A (2006). "Unbiased Recursive Partitioning: A Conditional Inference Framework." Journal of Computational and Graphical Statistics, 15(3), 651-674. doi:10.1198/106186006X133933

Zeileis A, Hothorn T, Hornik K (2008). "Model-Based Recursive Partitioning." Journal of Computational and Graphical Statistics, 17(2), 492-514. doi:10.1198/106186008X319331

Hothorn T, Zeileis A (2015). "partykit: A Modular Toolkit for Recursive Partytioning in R." Journal of Machine Learning Research, 16, 3905-3909. http://www.jmlr.org/papers/v16/hothorn15a

