Transformation Forests

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Abstract

Regression models for supervised learning problems with a continuous target are commonly understood as models for the conditional mean of the target given predictors. This notion is simple and therefore appealing for interpretation and visualisation. Information about the whole underlying conditional distribution is, however, not available from these models. A more general understanding of regression models as models for conditional distributions allows much broader inference from such models, for example the computation of prediction intervals. Several random forest-type algorithms aim at estimating conditional distributions, most prominently quantile regression forests (Meinshausen, 2006, JMLR). We propose a novel approach based on a parametric family of distributions characterised by their transformation function. A dedicated novel “transformation tree” algorithm able to detect distributional changes is developed. Based on these transformation trees, we introduce “transformation forests” as an adaptive local likelihood estimator of conditional distribution functions. The resulting models are fully parametric yet very general and allow broad inference procedures, such as the model-based bootstrap, to be applied in a straightforward way.

Keywords: random forest, transformation model, quantile regression forest, conditional distribution, conditional quantiles.

1. Introduction

Supervised machine learning plays an important role in many prediction problems. Based on a learning sample consisting of \( N \) pairs of target value \( y \) and predictors \( x \), one learns a rule \( r \) that predicts the status of some unseen \( Y \) via \( r(x) \) when only information about \( x \) is available. Both the machine learning and statistics communities differentiate between “classification problems”, where the target \( Y \) is a class label, and “regression problems” with conceptually continuous target observations \( y \). In binary classification problems with \( Y \in \{0,1\} \) the focus is on rules \( r \) for the conditional probability of \( Y \) being 1 given \( x \), more formally \( \Pr(Y = 1 \mid X = x) = r(x) \). Such a classification rule \( r \) is probabilistic in the sense that one cannot only predict the most probable class label but also assess the corresponding probability. This additional information is extremely valuable because it allows an assessment of the rules’ \( r \) uncertainty about its prediction. It is much harder to obtain such an assessment of uncertainty from most contemporary regression models, because the rule (or “regression function”) \( r \) typically describes the conditional expectation \( \mathbb{E}(Y \mid X = x) = r(x) \) but not the full predictive distribution of \( Y \) given \( x \). Thus, the prediction \( r(x) \) only contributes information about the mean of some unseen target \( Y \) but tells us nothing about other characteristics of its distribution. Without making additional restrictive assumptions, for example
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constant variances in normal distributions, the derivation of probabilistic statements from the regression function $r$ alone is impossible.

Contemporary random forest-type algorithms also strongly rely on the notion of regression functions $r$ describing the conditional mean $\mathbb{E}(Y \mid X = x)$ only (for example Biau et al. 2008; Biau 2012; Scornet et al. 2015), although the first random forest-type algorithm for the estimation of conditional distribution functions was published more than a decade ago (”bagging survival trees”, Hothorn et al. 2004). A similar approach was later developed independently by Meinshausen (2006) in his “quantile regression forests”. In contrast to a mean aggregation of cumulative hazard functions (Ishwaran et al. 2008) or densities (Criminisi et al. 2012), bagging survival trees and quantile regression forests are based on “nearest neighbour weights”. We borrow this term from Lin and Jeon (2006), where these weights were theoretically studied for the estimation of conditional means. The core idea is to obtain a “distance” measure based on the number of times a pair of observations is assigned to the same terminal node in the different trees of the forest. Similar observations have a high probability of ending up in the same terminal node whereas this probability is low for quite different observations. Then, the prediction for predictor values $x$ (either new or observed) is simply obtained as a weighted empirical distribution function (or Kaplan-Meier estimator in the context of right-censored target values) where those observations from the learning sample similar (or dissimilar) to $x$ in the forest receive high (or low/zero) weights, respectively. Although this aggregation procedure in the aforementioned algorithms is suitable for estimating predictive distributions, the underlying trees are not. The reason is that the ANOVA- or log-rank-type split procedures commonly applied are not able to deal with distributions in a general sense. Consequently, the splits favour the detection of changes in the mean – or have power against proportional hazards alternatives in survival trees. However, in general, they have very low power for detecting other patterns of heterogeneity (e.g., changes in variance) even if these can be explained by the predictor variables. A simple toy example illustrating this problem is given in Figure 1. Here, the target’s conditional normal distribution has a variance split at value $.5$ of a uniform $[0, 1]$ predictor. We fitted a quantile regression forest (Meinshausen 2006, 2017) to the 10,000 observations depicted in the figure along with ten additional independent uniformly distributed non-informative predictors (using 100 trees without random variable selection; see Appendix “Computational Details”). The true conditional 10% and 90% quantiles are not approximated very well by the quantile regression forest. In particular, the split at $.5$ does not play an important role in this model. Thus, although such an abrupt change in the distribution can be represented by a binary tree, the traditional ANOVA split criterion employed here was not able to detect this split.

To improve upon quantile regression forests and similar procedures in situations where changes in moments beyond the mean are important, we propose “transformation forests” for the estimation and prediction of conditional distributions for $Y$ given predictor variables $x$ and proceed in three steps. We first suggest to understand forests as adaptive local likelihood estimators (see Blomiarz et al. 2016, for a discussion of the special case of local linear regression). Second, we recap the most important features of the flexible and computationally attractive “transformation family” of distributions (Hothorn et al. 2014, 2017) which includes a variety of distribution families. Finally, we adapt the core ideas of “model-based recursive partitioning” (Zeileis et al. 2008, who also provide a review of earlier developments in this field) to this
transformation family and introduce novel algorithms for “transformation trees” and “transformation forests” for the estimation of conditional distribution functions which potentially vary in the mean and also in higher moments as a function of predictor variables $x$. In our small example in Figure 1, these novel transformation trees and forests were able to recover the true conditional distributions much more precisely than quantile regression forests. Owing to the fully parametric nature of the predictive distributions that can be obtained from these novel methods, model inference procedures, such as variable importances, independence tests or model-based resampling, can be formulated in a very general and straightforward way (Section 5). Some remarks on asymptotic properties are given in Section 6. The performance of transformation trees and forests is evaluated empirically on four artificial data generating processes and on survey data for body mass indices from Switzerland in Section 7. Details of the variable and split selection procedure in transformation trees as well as the corresponding theoretical complexity and empirical timings are discussed in Section 8.

2. Adaptive Local Likelihood Trees and Forests

We first deal with the unconditional distribution $P_Y$ of a target random variable $Y \in \mathcal{Y}$ and we restrict our attention to a specific probability model defined by the parametric family of distributions $P_{Y,\theta} = \{P_{Y,\theta} | \theta \in \Theta\}$ with parameters $\theta$ and parameter space $\Theta \subseteq \mathbb{R}^P$. With predictors $X = (X_1, \ldots, X_J) \in \mathcal{X}$ from some predictor sample space $\mathcal{X}$, our main interest is in the conditional distribution $P_{Y|X=x}$ and we assume that this conditional distribution is a member of the family of distributions introduced above, i.e., we assume that a parameter $\theta(x) \in \Theta$ exists such that $P_{Y|X=x} = P_{Y,\theta(x)}$. We call $\theta : \mathcal{X} \to \Theta$ the “conditional parameter function” and the task of estimating the conditional distributions $P_{Y|X=x}$ for all $x$ reduces to the problem of estimating this conditional parameter function.

From the probability model $P_{Y,\theta}$ we can derive the log-likelihood contribution $\ell_i : \Theta \to \mathbb{R}$ for each of $N$ independent observations $(y_i, x_i)$ from the learning sample for $i = 1, \ldots, N$. We propose and study a novel random forest-type estimator $\hat{\theta}_N^{\text{Forest}}$ of the conditional parameter function $\theta$ in the class of adaptive local likelihood estimators of the form

$$\hat{\theta}_N^N(x) := \arg\max_{\theta \in \Theta} \sum_{i=1}^N w_i^N(x) \ell_i(\theta); \quad x \in \mathcal{X} \tag{1}$$

where $w_i^N : \mathcal{X} \to \mathbb{R}^+$ is the “conditional weight function” for observation $i$ given a specific configuration $x$ of the predictor variables (which may correspond to an observation from the learning sample or to new data). This weight measures the similarity of the two distributions $P_{Y|X=x_i}$ and $P_{Y|X=x}$ under the probability model $P_{Y,\theta}$. The main idea is to obtain a large weight for observations $i$ which are “close” to $x$ in light of the model and essentially zero in the opposite case. The superscript $N$ indicates that the weight function may depend on the learning sample, and in fact the choice of the weight function $w_i^N$ is crucial in what follows.

Local likelihood estimation goes back to Brillinger (1977) in a comment to Stone (1977) and was the topic of Robert Tibshirani’s PhD thesis, published in Tibshirani and Hastie (1987).
Early regression models in this class were based on the idea of fitting polynomial models locally within a fixed smoothing window. Adaptivity of the weights refers to an $x$-dependent, non-constant smoothing window, i.e., different weighing schemes are applied in different parts of the predictor sample space $X$. An overview of local likelihood procedures was published by Loader (1999). Subsequently, we illustrate how classical maximum likelihood estimators, model-based trees, and model-based forests can be embedded in this general framework by choosing suitable conditional weight functions and plugging these into (1).

The unconditional maximum likelihood estimator is based on unit weights $w_{\text{ML},i}^N := 1$ not depending on $x$, i.e., all observations in the learning sample are considered to be equally “close”; thus

$$\hat{\vartheta}^N_{\text{ML}} := \arg \max_{\vartheta \in \Theta} \sum_{i=1}^{N} \ell_i(\vartheta).$$

In contrast, model-based trees can adapt to the learning sample by employing rectangular splits to define a partition $X = \bigcup_{b=1}^{B} B_b$ of the predictor sample space. Each of the $B$ cells then contains a different local unconditional model. More precisely, the conditional weight function $w_{\text{Tree},i}^N$ is simply an indicator for $x_i$ and $x$ being elements of the same terminal node so that only observations in the same terminal node are considered to be “close”. The weight and parameter functions are

$$w_{\text{Tree},i}^N(x) := \sum_{b=1}^{B} I(x \in B_b \land x_i \in B_b)$$

$$\hat{\vartheta}^N_{\text{Tree}}(x) := \arg \max_{\vartheta \in \Theta} \sum_{i=1}^{N} w_{\text{Tree},i}^N(x) \ell_i(\vartheta).$$

Thus, this essentially just picks the parameter estimate from the $b$-th terminal node which is associated with cell $B_b$,

$$\hat{\vartheta}_b^N = \arg \max_{\vartheta \in \Theta} \sum_{i=1}^{N} I(x_i \in B_b) \ell_i(\vartheta),$$

along with the corresponding conditional distribution $P_{Y,\hat{\vartheta}_b^N}$. Model-based recursive partitioning (MOB, Zeileis et al. 2008) is one representative of such a tree-structured approach.

A forest of $T$ trees is associated with partitions $X = \bigcup_{b=1}^{B_t} B_{tb}$ for $t = 1, \ldots, T$. The $b$-th terminal node of the $t$-th tree contains the parameter estimate $\hat{\vartheta}_b^N$ and the $t$-th tree defines the conditional parameter function $\hat{\vartheta}_{\text{Tree},t}^N(x)$. We define the forest conditional parameter function via “nearest neighbour” forest weights

$$w_{\text{Forest},i}^N(x) := \sum_{t=1}^{T} \sum_{b=1}^{B_t} I(x \in B_{tb} \land x_i \in B_{tb})$$

$$\hat{\vartheta}_{\text{Forest}}^N(x) := \arg \max_{\vartheta \in \Theta} \sum_{i=1}^{N} w_{\text{Forest},i}^N(x) \ell_i(\vartheta).$$
The conditional weight function \( w_{\text{Forest},i}^N \) counts how many times \( x_i \) and \( x \) are element of the same terminal node in each of the \( T \) trees, i.e., captures how “close” the observations are on average across the trees in the forest. Hothorn et al. (2004) first suggested these weights for the aggregation of \( T \) survival trees. The same weights have later been used by Lin and Jeon (2006) for estimating conditional means, by Meinshausen (2006) for estimating conditional quantiles and by Bloniarz et al. (2016) for estimating local linear models. An “out-of-bag” version only counts the contribution of the \( t \)-th tree for observation \( i \) when \( i \) was not used for fitting the \( t \)-th tree.

Forests relying on the aggregation scheme (3) model the conditional distribution \( P_{Y|X=x} \) for some configuration \( x \) of the predictors as \( P_{Y,\hat{\theta}_{\text{Forest}}^N(x)} \in P_{Y,\Theta} \). In this sense, such a forest is a fully specified parametric model with (in-bag or out-of-bag) log-likelihood

\[
\sum_{i=1}^N \ell_i \left( \hat{\theta}_{\text{Forest}}^N(x_i) \right)
\]

allowing a broad range of model inference procedures to be directly applied as discussed in Section 5. Although this core idea seems straightforward to implement, we unfortunately cannot pick our favourite tree-growing algorithm and mix it with some parametric model as two critical problems remain to be addressed in this paper. First, most of the standard tree-growing algorithms are not ready to be used for finding the underlying partitions because their variable and split selection procedures have poor power for detecting distributional changes which are not linked to changes in the mean as was illustrated by the simple toy example presented in the introduction. Therefore, a tailored tree-growing algorithm inspired by model-based recursive partitioning also able to detect changes in higher moments is introduced in Section 4.

The second problem is associated with the parametric families \( P_{Y,\Theta} \). Although, in principle, all classical probability models are suitable in this general framework, different parameterizations render unified presentation and especially implementation burdensome. We address this second problem by restricting our implementation to a novel transformation family of distributions. Theoretically, this family contains all univariate probability distributions \( P_Y \) and practically close approximations thereof. We highlight important aspects of this family and the corresponding likelihood function in the next section.

### 3. Transformation Models

A transformation model \( P(Y \leq y) = F_Y(y) = F_Z(h(y)) \) describes the distribution function of \( Y \) by an unknown monotone increasing transformation function \( h \) and some a priori chosen continuous distribution function \( F_Z \). We use this framework because simple, e.g., linear, transformation functions implement many of the classical parametric models whereas more complex transformation functions provide similar flexibility as models from the non-parametric world. In addition, discrete and continuous targets, also under all forms of random censoring and truncation, are handled in a unified way. As a consequence, our corresponding “transformation forests” will be applicable to a wide range of targets (discrete, continuous with or without censoring and truncation, counts, survival times) with the option to gradually move from simple to very flexible models for the conditional distribution functions \( P_{Y,\hat{\theta}_{\text{Forest}}^N(x)} \).

In more detail, let \( Z \sim P_Z \) denote an absolutely continuous random variable with density, distribution, and quantile functions \( f_Z, F_Z \) and \( F_Z^{-1} \), respectively. We furthermore assume
0 < F_Z(z) < \infty \forall z \in \mathbb{R} for a log-concave density \( F_Z \) as well as the existence of the first two derivatives of the density \( F_Z(z) \) with respect to \( z \), both derivatives shall be bounded. We do not allow any unknown parameters for this distribution. Possible choices include the standard normal, the standard logistic and the standard minimum extreme value distribution with distribution functions \( F_Z(z) = \Phi(z) \), \( F_Z(z) = F_{\text{SL}}(z) = (1 + \exp(-z))^{-1} \) and \( F_Z(z) = F_{\text{MEV}}(z) = 1 - \exp(-\exp(z)) \), respectively.

Let \( \mathcal{H} = \{ h : \mathcal{Y} \to \mathbb{R} \mid h(y_1) < h(y_2) \forall y_1 < y_2 \in \mathcal{Y} \} \) denote the space of all strictly monotone transformation functions. With the transformation function \( h \) we can write \( F_Y \) as \( F_Y(y \mid h) = F_Z(h(y)) \forall y \in \mathcal{Y} \) with density \( f_Y(y \mid h) \) and there exists a unique transformation function \( h = F_Z^{-1} \circ F_Y \) for all distribution functions \( F_Y \) (Hothorn et al. 2017). A convenient feature of characterising the distribution of \( Y \) by means of the transformation function \( h \) is that the likelihood for arbitrary measurements can be written and implemented in an extremely compact form.

For a given transformation function \( h \), the likelihood contribution of an observation \( y \in \mathbb{R} \) is given by the corresponding density

\[
\mathcal{L}(h \mid Y = y) = f_Z(h(y))h'(y).
\]

The likelihood for intervals \( (y_l, y_r] \subset \mathcal{Y} \) is, unlike in the above “exact continuous” case, defined in terms of the distribution function (Lindsey 1996), where one can differentiate between three special cases:

\[
\mathcal{L}(h \mid Y \in (y_l, y_r]) = \begin{cases} 
F_Z(h(y)) - F_Z(h(y_l)) & y \in (y_l, y_r] \text{ “interval-censored”} \\
1 - F_Z(h(y_l)) & y \in (y_l, \infty) \text{ “right-censored”} \\
F_Z(h(y_r)) & y \in (-\infty, y] \text{ “left-censored”}
\end{cases}
\]

For truncated observations in the interval \( (y_l, y_r] \subset \mathcal{Y} \), the above likelihood contribution has to be multiplied by the factor \( (F_Z(h(y_r)) - F_Z(h(y_l)))^{-1} \) when \( y_l < y < y_r \leq y_r \). A more detailed discussion of likelihood contributions to transformation models can be found in Hothorn et al. (2017).

We parameterise the transformation function \( h(y) \) as a linear function of its basis-transformed argument \( y \) using a basis function \( a : \mathcal{Y} \to \mathbb{R}^P \) such that \( h(y) = a(y)^\top \vartheta, \vartheta \in \mathbb{R}^P \). In the following, we will write \( h = a^\top \vartheta \) and assume that the true unknown transformation function is of this form. For continuous targets \( Y \) the parameterisation \( h(y) = a(y)^\top \vartheta \) needs to be smooth in \( y \), so any polynomial or spline basis is a suitable choice for \( a \). For the empirical experiments in Section 7 we employed Bernstein polynomials (for an overview see Farouki 2012) of order \( M \) \( (P = M + 1) \) defined on the interval \( [\bar{y}, \tilde{y}] \) with

\[
a_{\text{Bs},M}(y) = (M + 1)^{-1}(f_{\text{Be}(1,M+1)}(\bar{y}), \ldots, f_{\text{Be}(m,M-m+1)}(\bar{y}), \ldots, f_{\text{Be}(M+1,1)}(\bar{y}))^\top \in \mathbb{R}^{M+1}
\]

\[
h(y) = a_{\text{Bs},M}(y)^\top \vartheta = \sum_{m=0}^{M} \vartheta_m f_{\text{Be}(m+1,M-m+1)}(\bar{y})/((M + 1))
\]

\[
h'(y) = a'_{\text{Bs},M}(y)^\top \vartheta = \sum_{m=0}^{M-1} (\vartheta_{m+1} - \vartheta_m) f_{\text{Be}(m+1,M-m)}(\bar{y}) M/((M + 1)(\bar{y} - \bar{y}))
\]

where \( \bar{y} = (y - \bar{y})/(\bar{y} - \bar{y}) \in [0, 1] \) and \( f_{\text{Be}(m,M)} \) is the density of the Beta distribution with parameters \( m \) and \( M \). This choice is computationally attractive because strict monotonicity
can be formulated as a set of $M$ linear constraints on the parameters $\vartheta_m < \vartheta_{m+1}$ for all $m = 0, \ldots, M$ (Curtis and Ghosh 2011).

The distribution family $\mathbb{P}_{Y; \Theta} = \{F_Z \circ a^\top \vartheta \mid \vartheta \in \Theta\}$ that transformation forests are based upon is called transformation family of distributions with parameter space $\Theta = \{\vartheta \in \mathbb{R}^P \mid a^\top \vartheta \in \mathcal{H}\}$ and transformation functions $a^\top \vartheta \in \mathcal{H}$. This family encompasses a wide variety of densities capturing different locations and shapes (including scale and skewness), see Figure 6 for an illustration of different body mass index distributions. The log-likelihood contribution for an observation $y_i \in \mathbb{R}$ is now the log-density of the transformation model $\ell_i(\vartheta) = \log(f_Z(a(y_i)^\top \vartheta)) + \log(a'(y_i)^\top \vartheta)$.

4. Transformation Trees and Forests

Conceptually, the model-based recursive partitioning algorithm (Zeileis et al. 2008) for tree induction starts with the maximum likelihood estimator $\hat{\vartheta}_{\text{ML}}^N$. Deviations from such a given model that can be explained by parameter instabilities due to one or more of the predictors are investigated based on the score contributions. The novel “transformation trees” suggested here rely on the transformation family $\mathbb{P}_{Y; \Theta} = \{F_Z \circ a^\top \vartheta \mid \vartheta \in \Theta\}$ whose score contributions $s$ have relatively simple and generic forms. The score contribution of an “exact continuous” observation $y \in \mathbb{R}$ from an absolutely continuous distribution is given by the gradient of the log-density with respect to $\vartheta$

$$s(\vartheta \mid Y = y) = a(y) \frac{f'_Z(a(y)^\top \vartheta)}{f_Z(a(y)^\top \vartheta)} + \frac{a'(y)}{a'(y)^\top \vartheta}.$$ 

For an interval-censored observation $(y, \bar{y}]$ the score contribution is

$$s(\vartheta \mid Y \in (y, \bar{y}]) = \frac{f_Z(a(\bar{y})^\top \vartheta)a(\bar{y}) - f_Z(a(y)^\top \vartheta)a(y)}{F_Z(a(\bar{y})^\top \vartheta) - F_Z(a(y)^\top \vartheta)}.$$ 

Under truncation to the interval $(y_l, y_r] \subset \mathcal{Y}$, one needs to subtract the term $s(\vartheta \mid Y \in (y_l, y_r])$ from the score function.

With the transformation model and thus the likelihood and score function being available, we start our tree induction with the global model $\mathbb{P}_{Y; \hat{\vartheta}_{\text{ML}}^N}$. The hypothesis of all observations $i = 1, \ldots, N$ coming from this model can be written as the independence of the $P$-dimensional score contributions and all predictors, i.e.,

$$H_0 : s(\hat{\vartheta}_{\text{ML}}^N \mid Y) \perp X.$$ 

This hypothesis can be tested either using asymptotic M-fluctuation tests (Zeileis et al. 2008) or permutation tests (Hothorn et al. 2006b; Zeileis and Hothorn 2013) with appropriate multiplicity adjustment depending on the number of predictors. Rejection of $H_0$ leads to the implementation of a binary split in the predictor variable with most significant association to the score matrix; algorithmic details are discussed in Section 8. Unbiasedness of a model-based tree with respect to variable selection is a consequence of splitting in the variable of highest association to the scores where association is measured by the marginal multiplicity-adjusted p-value (for details see Hothorn et al. 2006b; Zeileis et al. 2008, and Section 8). The
procedure is recursively iterated until $H_0$ cannot be rejected. The result is a partition of the sample space $\mathcal{X} = \bigcup_{b=1,\ldots,B} B_b$.

Based on the “transformation trees” introduced here, we construct a corresponding random forest-type algorithm as follows. A “transformation forest” is an ensemble of $T$ transformation trees fitted to subsamples of the learning sample and, optionally, a random selection of candidate predictors available for splitting in each node of the tree. The result is a set of $T$ partitions of the predictor sample space. The transformation forest conditional parameter function is defined by its nearest neighbour forest weights (3).

The question arises how the order $M$ of the parameterisation of the transformation function $h$ via Bernstein polynomials affects the conditional distribution functions $P_{Y, \hat{\vartheta}_N^{\text{Tree}}}(x)$ and $P_{Y, \hat{\vartheta}_N^{\text{Forest}}}(x)$. On the one hand, the basis $a_{B_s,1}$ with $F_Z = \Phi$ only allows linear transformation functions of a standard normal and thus our models for $P_{Y|X=x}$ are restricted to the normal family, however, with potentially both mean and variance depending on $x$ as the split criterion in transformation trees is sensitive to changes in both mean and variance. This most simple parameterisation leads to transformation trees and forests from which both the conditional mean and the conditional variance can be inferred. Using a higher order $M$ also allows modelling non-normal distributions. In the extreme case with $M = N-1$ the unconditional distribution function $F_Z(a_{B_s,M}(y)^T \vartheta)$ interpolates the unconditional empirical cumulative distribution function of the target. With $M > 1$, the split criterion introduced in this section is able to detect changes beyond the second moment and, consequently, also higher moments of the conditional distributions $P_{Y|X=x}$ may vary with $x$. An empirical comparison of transformation trees and forests with linear ($M = 1$) and nonlinear ($M > 1$) transformation function can be found in Section 7. Additional empirical properties of transformation models with larger values of $M$ are discussed in Hothorn (2018a).

5. Transformation Forest Inference

In contrast to other random forest regression models, a transformation forest is a fully-specified parametric model. Thus, we can derive all interesting model inference procedures from well-defined probability models and do not need to fall back to heuristics. Predictions from transformation models are distributions $P_{Y, \hat{\vartheta}_N^{\text{Forest}}}(x)$ and we can describe these on the scale of the distribution, quantile, density, hazard, cumulative hazard, expectile, and any other characterising functions. By far not being comprehensive, we introduce prediction intervals, a unified definition of permutation variable importance, the model-based bootstrap and a test for global independence in this section.

5.1. Prediction Intervals and Outlier Detection

For some yet unobserved target $Y$ under predictors $x$, a two-sided $(1 - \alpha)$ prediction interval for $Y \mid X = x$ and some $\alpha \in (0, 0.5)$ can be obtained by numerical inversion of the conditional distribution $P_{Y, \hat{\vartheta}_N^{\text{Forest}}}(x)$, for example via

$$PI_{\alpha}(x \mid \hat{\vartheta}_N^{\text{Forest}}) = \{y \in Y \mid \alpha/2 < P_{Y, \hat{\vartheta}_N^{\text{Forest}}}(x)(y) \leq 1 - \alpha/2\}$$
with the property
\[ P_{Y|X=x} (\text{PI}_\alpha (x | \theta)) = 1 - \alpha. \]

The empirical level \( P_{Y|X=x} (\text{PI}_\alpha (x | \hat{\theta}_{\text{Forest}}^N)) \) depends on how well the parameters \( \theta(x) \) are approximated by the forest estimate \( \hat{\theta}_{\text{Forest}}^N(x) \). If for some observation \((y_i, x_i)\) the corresponding prediction interval \( \text{PI}_\alpha (x_i | \hat{\theta}_{\text{Forest}}^N) \) excludes \( y_i \), one can (at level \( \alpha \)) suspect this observed target of being an outlier.

### 5.2. Permutation Variable Importance

The importance of a variable is defined as the amount of change in the risk function when the association between one predictor variable and the target is artificially broken. Permutation variable importances permute one of the predictors at a time (and thus also break the association to the remaining predictors, see Strobl et al. 2008). The risk function for transformation forests is the negative log-likelihood, thus a universally applicable formulation of variable importance for all types of target distributions in transformation forests is

\[
\text{VI}(j) = T^{-1} \sum_{t=1}^{T} \left( \sum_{i=1}^{N} -\ell_i \left( \hat{\theta}_{\text{Tree},t}^N(x_i) \right) - \sum_{i=1}^{N} -\ell_i \left( \hat{\theta}_{\text{Tree},t}^N(x_i^{(j)}) \right) \right)
\]

where the \( j \)-th variable was permuted in \( x_i^{(j)} \) for \( i = 1, \ldots, N \).

### 5.3. Model-Based Bootstrap

We suggest the model-based, or “parametric”, bootstrap to assess the variability of the estimated forest conditional parameter function \( \hat{\theta}_{\text{Forest}}^N \) as follows. First, we fit a transformation forest and sample new target values \( \tilde{y}_i \sim P_{Y, \hat{\theta}_{\text{Forest}}^N(x_i)} \) for each observation \( i = 1, \ldots, N \) from this transformation forest. For these \( i = 1, \ldots, N \) pairs of artificial targets and original predictors \((\tilde{y}_i, x_i)\), we refit the transformation forest. This procedure of sampling and refitting is repeated \( k = 1, \ldots, K \) times. The resulting \( K \) conditional parameter functions \( \hat{\theta}_{\text{Forest},k}^N, k = 1, \ldots, K \) are a bootstrap sample from the distribution of conditional parameter functions assuming the initial \( \hat{\theta}_{\text{Forest}}^N \) was the true conditional parameter function. The bootstrap distribution of \( \hat{\theta}_{\text{Forest},k}^N(x) \) or functionals thereof can be used to study their variability or to derive bootstrap confidence intervals (Efron and Tibshirani 1993) for parameters \( \theta(x) \) or other quantities, such as conditional quantiles.

### 5.4. Independence Likelihood-Ratio Test

The first question many researchers have is “Is there any signal in my data?”, or, in other words, is the target \( Y \) independent of all predictors \( X \)? Classical tests, such as the \( F \)-test in a linear model or multiplicity-adjusted univariate tests, have very low power against complex alternatives, i.e., in situations where the impact of the predictors is neither linear nor marginally visible. Because transformation forests can potentially detect such structures, we propose a likelihood-ratio test for the null \( H_0 : Y \perp X \). This null hypothesis is identical to \( H_0 : P_Y = P_{Y|X=x} \forall x \in X \) and reads \( H_0 : P_{Y,\theta} = P_{Y,\theta(x)} \forall x \in X \), or even simpler, \( H_0 : \theta(x) \equiv \theta \) for the class of models we are studying. Under the null hypothesis, the
unconditional maximum likelihood estimator $\hat{\vartheta}_{ML}^N$ would be optimal. It therefore makes sense to compare the log-likelihoods of the unconditional model with the log-likelihood of the transformation forest using the log-likelihood ratio statistic

$$\log \text{LR} = \sum_{i=1}^{N} \ell_i \left( \hat{\vartheta}_{\text{Forest}}^N(x_i) \right) - \sum_{i=1}^{N} \ell_i \left( \hat{\vartheta}_{ML}^N \right)$$

Under $H_0$ we expect small differences and under the alternative we expect to see larger log-likelihoods of the transformation forest. The null distribution of such likelihood-ratio statistics is hard to assess analytically but can be easily approximated by the model-based bootstrap (early references include McLachlan 1987; Beran 1988). We first estimate the unconditional model $\mathbb{P}_Y, \hat{\vartheta}_{ML}^N$ and, in a second step, draw $k = 1, \ldots, K$ samples from this model $\mathbb{P}_Y, \hat{\vartheta}_{ML}^N$ of size $N$, i.e., we sample from the unconditional model, in this sense treating $\hat{\vartheta}_{ML}^N$ as the “true” parameter. In the $k$-th sample the predictors are identical to the those in the learning sample and only the target values are replaced. For each of these $k$ samples we refit the transformation forest and obtain $\hat{\vartheta}_{\text{Forest},k}^N(x_i)$. Based on this model we compute the log-likelihood ratio statistic

$$\log \text{LR}_k = \sum_{i=1}^{N} \ell_{i,k} \left( \hat{\vartheta}_{\text{Forest},k}^N(x_i) \right) - \sum_{i=1}^{N} \ell_{i,k} \left( \hat{\vartheta}_{ML}^N \right)$$

where $\ell_{i,k}$ is the log-likelihood contribution by the $i$-th observation from the $k$-th bootstrap sample. The $p$-value for $H_0$ is now $K^{-1} \sum_k I(\log \text{LR}_k > \log \text{LR})$. The size of this test in finite samples depends on the performance of transformation forests under $H_0$ and its power on the ability of transformation forests to detect non-constant conditional parameter functions $\vartheta(x)$. Empirical evidence for a moderate overfitting behaviour and a high power for detecting distributional changes are reported in Section 7.

6. Theoretical Evaluation

The theoretical properties of random forest-type algorithms are a contemporary research problem and we refer to Biau and Scornet (2016) for an overview. In this section we discuss how these developments relate to the asymptotic behaviour of transformation trees and transformation forests.

For $\vartheta(x) \equiv \vartheta$ the maximum likelihood estimator ($w_i \equiv 1$) is consistent and asymptotically normal (Hothorn et al. 2017). In the non-parametric setup, i.e., for arbitrary distributions $\mathbb{P}_Y$, Hothorn et al. (2014) provide consistency results in the class of conditional transformation models. Based on these results, consistency and normality of the local likelihood estimator for an a priori known partition $X = \bigcup_{b=1,\ldots,B} B_b$ is guaranteed as long as the sample size tends to infinity in all cells $b$.

If the partition (transformation trees) or the nearest neighbour weights (transformation forests) are estimated from the data, established theoretical results on random forests (Breiman 2004; Lin and Jeon 2006; Meinshausen 2006; Biau et al. 2008; Biau 2012; Scornet et al. 2015) provide a basis for the analysis of transformation forests. Lin and Jeon (2006) first analysed random forests for estimating conditional means with adaptive nearest neighbours weights,
where estimators for the conditional mean of the form

$$\hat{E}_N(Y \mid X = x) = \frac{\sum_{i=1}^N w_{\text{Forest},i}(x) Y_i}{\sum_{i=1}^N w_{\text{Forest},i}(x)}$$

were shown to be consistent in non-adaptive random forests

$$E_{Y \mid X = x} \left( E(Y \mid X = x) - \hat{E}_N(Y \mid X = x) \right)^2 \to 0$$
as $N \to \infty$. Meinshausen (2006) showed a Glivenko-Cantelli-type result for conditional distribution functions

$$\hat{P}_N(Y \leq y \mid X = x) = \hat{E}_N(I(Y \leq y) \mid X = x) = \frac{\sum_{i=1}^N w_{\text{randomForest},i}(x) I(Y_i \leq y)}{\sum_{i=1}^N w_{\text{randomForest},i}(x)}$$

where the weights are obtained from Breiman and Cutler’s original random forest implementation (Breiman 2001).

In order to understand the applicability of these results to transformation forests, we define the expected conditional log-likelihood given $x$ for a fixed set of parameters $\theta$ as

$$\ell(\theta \mid X = x) := E_{Y \mid X = x} \ell(\theta, Y), \quad \ell(\theta, Y_i) = \ell_i(\theta)$$

where $\ell(\theta, Y_i) = \ell_i(\theta)$ is the likelihood contribution by some observation $Y_i$. By definition, the true unknown parameter $\theta(x)$ has minimal expected risk and thus maximises the expected log-likelihood, i.e.,

$$\theta(x) = \arg \max_{\theta \in \Theta} \ell(\theta \mid X = x).$$

Our random forest-type estimator of the expected conditional log-likelihood given $x$ for a fixed set of parameters $\theta$ is now

$$\hat{\ell}_N(\theta \mid X = x) = \frac{\sum_{i=1}^N w_{\text{Forest},i}(x) \ell(\theta, Y_i)}{\sum_{i=1}^N w_{\text{Forest},i}(x)}.$$

Under the respective conditions on the distribution of $X$ and the joint distribution of $Y, X$ given by Lin and Jeon (2006), Biau and Devroye (2010), or Biau (2012), this estimator is consistent for all $\theta \in \Theta$

$$E_{Y \mid X = x} \left( \ell(\theta \mid X = x) - \hat{\ell}_N(\theta \mid X = x) \right)^2 \to 0$$

(the result being derived for non-adaptive random forests). This result gives us consistency of the conditional log-likelihood function

$$\hat{\ell}_N(\theta \mid X = x) \overset{p}{\to} \ell(\theta \mid X = x) \quad \forall \theta \in \Theta.$$

The forest conditional parameter function $\hat{\theta}_N^{\text{Forest}}(x)$ is consistent when

$$P_{\theta}(\hat{\ell}_N(\theta_1 \mid X = x) < \hat{\ell}_N(\theta \mid X = x)) \overset{p}{\to} 1$$
as $N \to \infty$ for all $\vartheta_1$ in a neighbourhood of $\vartheta$. The result $\hat{\vartheta}_{\text{forest}}^N(x) \xrightarrow{P} \vartheta(x)$ can be shown under the assumptions regarding $\ell$ given by Hothorn et al. (2017), especially continuity in $\vartheta$. Because the conditional log-likelihood $\hat{\ell}^N(\vartheta \mid X = x)$ is a conditional mean-type estimator of a transformed target $Y$, future theoretical developments in the asymptotic analysis of more realistic random forest-type algorithms based on nearest neighbour weights will directly carry over to transformation forests.

It is worth noting that some authors studied properties of random forests in regression models of the form $Y = r(x) + \varepsilon$ where the conditional variance $\mathbb{V}(Y \mid X = x)$ does not depend on $x$. This is in line with the ANOVA split criterion implemented in Breiman and Cutler’s random forests (Breiman 2001). The split procedure applied in transformation trees is, as will be illustrated in the next section, able to detect changes in higher moments. Thus, transformation forests might be a way to relax the assumption of additivity of signal and noise in the future.

### 7. Empirical Evaluation

Transformation forests were evaluated empirically, comparing this novel member of the random forest family to established procedures using artificial data generating processes. The data scenarios controlled the variation of several properties of interest: type of conditional parameter function, types of effect, and model complexity in low and high dimensions. The corresponding hypotheses to be assessed are:

**H1: Type of Conditional Parameter Regression.**

**H1a: Tree-Structured Conditional Parameter Function.** Transformation trees and forests are able to identify subgroups associated with different transformation models, i.e., subgroups formed by a recursive partition (or tree) in predictor variables $x$ corresponding to different parameters and thus different conditional distributions $\mathbb{P}_{Y \mid X = x}$.

**H1b: Non-Linear Conditional Parameter Function.** Transformation forests are able to identify conditional distributions $\mathbb{P}_{Y \mid X = x}$ whose parameters depend on predictor variables $x$ in a smooth non-linear way.

**H2: Type of Effect.**

**H2a: No Effect.** In a non-informative scenario with $\mathbb{P}_{Y \mid X = x} = \mathbb{P}_Y$ (i.e., mean and all higher moments constant) transformation trees perform as good as the unconditional maximum likelihood estimator. Thus, there is no (pronounced) overfitting.

**H2b: Location Only.** Transformation trees and forests perform as good as classical regression trees and forests when higher moments of the conditional distribution $\mathbb{P}_{Y \mid X = x}$ are constant.

**H2c: Unlinked Location and Scale.** Transformation trees and forests outperform classical regression trees and forests when higher moments of the conditional distribution $\mathbb{P}_{Y \mid X = x}$ are varying in a way that is not linked to variations in the mean.

**H2d: Linked Location and Scale.** Transformation trees and forests perform as good as classical regression trees and forests when higher moments of the conditional distribution $\mathbb{P}_{Y \mid X = x}$ are varying but in a way that is linked to the mean.
H3: Model Complexity.

\[ P = 2: \] Transformation trees and forests with linear transformation function \( h \), i.e., with \( P = 2 \) parameters, perform best for conditionally normal target variables. Transformation trees and forests with non-linear transformation function \( h \) perform slightly worse in this situation.

\[ P = 6: \] Transformation trees and forests with non-linear transformation function \( h \), i.e., with \( P = 6 \) parameters of a Bernstein polynomial of order five, outperform transformation trees and forests with linear transformation function for conditionally non-normal target variables.

H4: Dimensionality. Transformation forests stabilise transformation trees in the presence of high-dimensional non-informative predictor variables.

7.1. Data Generating Processes

Two data generating processes corresponding to H1a and H1b were studied. The first problem implements simple binary splits in the conditional mean and/or conditional variance of a normal target allowing a direct comparison of the split criteria employed by classical and transformation trees. The second problem is inspired by the “Friedman 1” benchmark problem (Friedman 1991), and implements smooth non-linear conditional mean and variance functions for normal targets, in order to provide a more complex and more realistic scenario.

Tree-Structured Conditional Parameter Function (H1a) The conditional normal target

\[ Y \mid X = x \sim \mathcal{N} \left( \mu_{\text{Tree}}(x), \sigma_{\text{Tree}}(x)^2 \right) \] (5)

depends on tree-structured conditional mean and variance functions \( \mu(x) \) and \( \sigma(x)^2 \) according to four different setups (corresponding to hypotheses H2a–c):

| Hypothesis | \( \mu_{\text{Tree}}(x) \) | \( \sigma_{\text{Tree}}(x) \) |
|------------|----------------|----------------|
| H2a        | 0              | 1              |
| H2b        | \( I(x_1 > .5) \) | 1              |
| H2c        | 0              | \( 1 + I(x_2 > .5) \) |
| H2d        | \( I(x_1 > .5) \) | \( 1 + I(x_2 > .5) \) |

All predictors \( X = (X_1, \ldots, X_7) \) are independently uniform on [0, 1] in the low-dimensional case (two informative and five noise variables) and \( X = (X_1, \ldots, X_{52}) \) in the high-dimensional case (two informative and 50 noise variables, H4).

For the evaluation of hypothesis H2d we studied the same setup as above but for conditionally log-normal targets with

\[ Y' = \exp(Y). \] (6)

Here, the conditional mean of the target variable \( Y' \) depends both on the underlying conditional mean \( \mu(x) \) of \( Y \) and the corresponding conditional variance \( \sigma(x)^2 \):

\[ \mathbb{E}(Y' \mid X = x) = \exp(\mu(x) + \sigma(x)^2/2) \]
It is important to note that the true transformation function \( h \) in model (6) is a scaled and shifted log-transformation. Unlike the true linear transformation function \( h \) in model (5), which can be exactly fitted by the linear and Bernstein parameterisations of the transformation function in transformation trees and forests, the true log-transformation cannot be approximated well by the basis functions \( a \). Therefore, no competitor in this simulation experiment is able to exactly recover the true data generating process.

Non-Linear Conditional Parameter Function (H1b) The data generating process

\[
Y \mid X = x \sim N\left(\mu_{\text{Nonlin}}(x), \sigma_{\text{Nonlin}}(x)^2\right)
\]

with all predictors \( X = (X_1, \ldots, X_{15}) \) from independent uniform distributions on \([0, 1]\) in the low-dimensional case (ten informative and five noise variables) and \( X = (X_1, \ldots, X_{60}) \) in the high-dimensional case (ten informative and 50 noise variables, H4) is inspired by the “Friedman 1” benchmarking problem (Friedman 1991). This original benchmark problem is conditional normal with a conditional mean function depending on five uniform predictor variables

\[
\text{Friedman1}(x_1, x_2, x_3, x_4, x_5) = 10 \sin(\pi x_1 x_2) + 20(x_3 - .5)^2 + 10 x_4 + 5 x_5
\]

and constant variance. For our experiments, we scaled the output of Friedman1 to the \([-1.5, 1.5]\) interval and denote this scaled function as Friedman1*. Model (7) is conditionally normal with potentially non-constant conditional mean function

\[
\mu_{\text{Nonlin}}(x) = \text{Friedman1}^*(x_1, x_2, x_3, x_4, x_5)
\]

and potentially non-constant conditional variance function

\[
\sigma_{\text{Nonlin}}(x) = \exp(\text{Friedman1}^*(x_6, x_7, x_8, x_9, x_{10}))^2.
\]

The latter function is based on an additional set of five uniformly distributed predictor variables and thus the conditional mean and variance function are not linked (H2c).

Again, we considered all setups corresponding to H2a–c and H4, including the non-informative case with constant mean and variance:

| Hypothesis | \( \mu_{\text{Nonlin}}(x) \) | \( \sigma_{\text{Nonlin}}(x) \) |
|------------|-----------------|-----------------|
| H2a        | 0               | 1               |
| H2b        | \text{Friedman1}^*(x_1, x_2, x_3, x_4, x_5) | 1               |
| H2c        | 0               | \exp(\text{Friedman1}^*(x_6, x_7, x_8, x_9, x_{10})) |
| H2c        | \text{Friedman1}^*(x_1, x_2, x_3, x_4, x_5) | \exp(\text{Friedman1}^*(x_6, x_7, x_8, x_9, x_{10})) |

Hypothesis H2d for non-linear conditional parameter functions (H1b) was studied in the log-normal model

\[
Y' = \exp(Y).
\]
7.2. Competitors

For testing the hypotheses H1–H4, we compared the performance of transformation trees and forests with linear and non-linear transformation functions \( h \) to the performance of conditional inference trees (Hothorn et al. 2006b) and conditional inference forests (Strobl et al. 2007) as representatives of unbiased recursive partitioning and to Breiman and Cutler’s random forests (Breiman 2001) as an representative of exhaustive search procedures. In more detail, we compared the performance of the following methods:

**CTree:** Conditional inference trees with internal stopping by default parameters.

**TTree:** Transformation trees, either with linear \((P = 2)\) parameters or non-linear \((P = 6)\) parameters of a Bernstein polynomial) transformation functions. Tree-growing parameters are identical to those from CTree.

**CForest:** Conditional inference forests with \(\text{mtry}\) equal to one third of the number of predictor variables. Trees were grown without internal stopping until sample size constraints were met.

**RForest:** Breiman and Cutler’s random forests with tree-growing parameters analogous to CForest (i.e., same \(\text{mtry}\) and stopping based on sample size constraints).

**TForest:** Transformation forests, either with linear \((P = 2)\) or non-linear \((P = 6)\) transformation functions, and tree-growing parameters analogous to CForest and RForest.

See Table 1 for a schematic overview of all competitors and Appendix “Computational Details” for the exact tree-growing parameter specifications.

In order to allow a fair comparison on the same scale, trees and forests obtained from the classical methods, i.e., conditional inference trees and forests and Breiman and Cutler’s random forests, were used to estimate conditional parameter functions (2) and (3) in the same way as for transformation trees and forests: We first fitted trees and forests using the reference implementations of the corresponding methods and, second, computed the corresponding conditional weight functions, which allowed estimation of conditional parameter functions \(\vartheta_N^{\text{CTree}}, \vartheta_N^{\text{CForest}}, \) and \(\vartheta_N^{\text{RForest}}\) in the third step. It should be noted that the combination of Breiman and Cutler’s random forests with transformation models in our RForest variant is conceptually very similar to quantile regression forests. Meinshausen (2006, 2017) uses Breiman and Cutler’s random forest to build the trees. The only difference to our RForest variant is that aggregation in quantile regression forests takes place via the weighted empirical conditional cumulative distribution function with weights \(w_{\text{randomForest}}^N\), see Formula (4), instead of the application of a smooth conditional distribution function corresponding to a transformation model.

[Table 1 about here.]

7.3. Performance Measures

The primary performance measure is the out-of-sample log-likelihood because it assesses the whole predicted distribution in a “proper” way (Gneiting and Raftery 2007). To adjust
for sampling variation, the log-likelihood of the true data generating process is employed as the reference measure. More precisely, the negative log-likelihood difference, that is the negative log-likelihood of a competitor minus the negative log-likelihood of the true data generating process, was evaluated for the $N = 250$ observations of the validation sample. Conditional medians and prediction intervals are of additional interest and we also compared their performance by the out-of-sample check risk corresponding to the 10%, 50% (absolute error) and 90% quantiles in reference to the true data generating process. A direct comparison of coverage and lengths of prediction intervals is not considered as it would only be valid or useful for a given configuration of the predictor variables. This is termed “conditional coverage” vs. “sample coverage” in Mayr et al. (2012) or considered as maximising forecast sharpness only subject to calibration in the proper scoring rules literature (Gneiting et al. 2007).

7.4. Results: Tree-Structured Conditional Parameter Function (H1a)

Given the type of conditional parameter function (here: tree, H1a) all other properties of the data generating process are varied and assessed, summarising the results with parallel coordinate displays and superimposed boxplots of the negative log-likelihood differences (see Figure 2). These were obtained from 100 pairs of learning samples (size $N = 250$) and validation samples, using a normal dependent variable in the first step. This allows to assess the type of effect (mean and/or higher moments) in the rows of the panels (H2a–c), the dimensionality (H4) in the columns of the panels, and the complexity (H3, $P = 2$ vs. 6) along the $x$-axes.

In the situation where all predictor variables were non-informative (H2a, top row of Figure 2), CTree ($P = 2$) and TTree ($P = 2$) were most resistant to overfitting; this effect is due to the test-based internal stopping of the unbiased tree methods compared here. TTree ($P = 6$) with non-linear transformation function had slightly larger negative log-likelihood differences due to the increased model complexity (H3). Moreover, if model complexity is further increased by considering forests instead of trees, all random forest variants exhibit some more pronounced overfitting behaviour.

Under the simple change in the mean (H2b, second row in Figure 2), CTree ($P = 2$) and TTree ($P = 2$) were able to detect this split best. TTree ($P = 6$) and all random forest variants performed less well in this situation. A variance change (H2c, third row in Figure 2) lead to smallest negative log-likelihood difference and thus superior performance for all transformation trees and forests as compared to the trees and forests splitting only based on the mean. TTree ($P = 2$) performed best while none of the classical procedures seemed to be able to properly pick up this variance signal. The aggregation of multiple transformation trees lead to decreased performance, this effect was also visible in Figure 1 (which was based on the same data generating process (5)).

When changes in both mean and variance were present (H2c, fourth row in Figure 2), transformation forests with linear transformation function TForest ($P = 2$) performed as good as the corresponding TTree in the low-dimensional setup but better than all other procedures in the high-dimensional setup with 50 non-informative variables (H4). This effect might be due to a too restrictive inference-based early stopping in TTree. TTree ($P = 6$) showed some extreme outliers (H3, visible in the parallel coordinates in Figure 2) which were due to convergence problems. The corresponding transformation forests TForest ($P = 6$), however, did
not experience such problems and thus seemed to stabilise the trees.

In summary, the results with respect to our hypotheses were:

**H1a:** Transformation trees reliably recover tree-structured conditional parameter functions in both mean and variance.

**H2a:** Transformation trees are rather robust to overfitting when there is no effect while transformation forests (like all other random forests) exhibit some overfitting.

**H2b:** Transformation trees and forests perform comparably to their classical counterparts.

**H2c:** Transformation trees and forests outperform their classical counterparts if there are only variance effects or variance effects that are not linked to the mean.

**H3:** For normal responses transformation trees and forests with linear transformation function \((P = 2)\) consistently perform better than the more complex Bernstein polynomials \((P = 6)\).

**H4:** Transformation forests stabilise the transformation trees in high-dimensional settings.

[Figure 2 about here.]

As a next step, the same simulation experiments were considered using a log-normal target variable instead of the normal variable employed above. Figure 3 depicts the negative log-likelihood differences for this setup, based on 100 learning samples of size \(N = 2500\). Using this highly skewed distribution affects the results regarding the following two hypotheses:

**H3** All models with complexity \(P = 2\) are clearly not appropriate anymore as they cannot capture the skewness. Consequently, all models based on the more flexible Bernstein polynomials with \(P = 6\) outperform all other methods.

**H2d** The classic RForest \((P = 6)\), i.e., the combination of Breiman and Cutler’s random forests with a subsequent flexible transformation model, performs almost on par with transformation trees and forests even when there are changes in the variance only. The reason is that any changes in the variance are always also linked to changes in the mean due to the skewness of the distribution.

[Figure 3 about here.]

Qualitatively the same conclusions can be drawn when assessing the competing methods based on predictions of the conditional 10% quantiles (Figure 10 and 13 for normal and log-normal targets, respectively), 50% quantiles (Figure 11 and 14), and 90% quantiles (Figure 12 and 15). However, the differences are less pronounced for the 50% quantiles (medians, corresponding to the absolute errors). Note also that combining predictions of 10% and 90% quantiles amounts to 80% prediction intervals.

By and large, all empirical results in this section conformed with our hypotheses H1–4, suggesting a stable behaviour of transformation trees and forests, especially with appropriate linear transformation function for normal targets, in these very simple situations. The next
section proceeds to a less idealised scenario with non-linear conditional parameter functions defining mean and/or variance.

7.5. Results: Non-Linear Conditional Parameter Function (H1b)

The same hypotheses were assessed as in the previous section but for non-linear Friedman1-type conditional parameter functions instead of the tree-structured functions considered previously. More specifically, Figures 4 and 8 depict the negative log-likelihood differences based on 100 learning samples with normally-distributed targets ($N = 500$) and log-normally-distributed targets ($N = 2500$), respectively. We summarise the results as follows.

**H1b**: When a signal was present (rows 2–4), all random forest variants outperformed single trees under normality. Under non-normality, this still holds for the random forest variants combined with flexible models ($P = 6$).

**H2a**: When there is no effect (top rows), CTree ($P = 2$) and TTree ($P = 2$) showed best resistance to overfitting under normality. Under non-normality, TTree ($P = 6$) still shows this behavior but the corresponding forests also perform similarly well.

**H2b**: All forest variants performed similarly well when predictor variables only had an effect on the mean (second rows).

**H2c**: Under normality, transformation forests performed best when some of the predictor variables also affected the variance (rows 3–4), where the classical procedures were not able to capture these changes appropriately.

**H2d**: Under non-normality, transformation forests (with $P = 6$) still perform best (rows 3–4). However, the classical RForest also performs well albeit with a much larger variance than TForest.

**H3**: Under non-normality, all trees and forests combined with flexible Bernstein polynomials ($P = 6$) clearly outperform all other methods. Under normality, the flexible models with $P = 6$ were sometimes slightly worse than the $P = 2$ models but often also a little bit better.

**H4**: In many situations the picture in low-dimensional settings (left column) is quite similar to that in high-dimensional scenarios (right column). However, sometimes it can be seen that transformation forests stabilise transformation trees in the presence of high-dimensional non-informative predictor variables.

As before, qualitatively the same patterns could be observed for the corresponding 10%, 50%, and 90% check risks (Figures 16–18 and Figures 19–21, respectively) and thus prediction intervals. In summary, our hypotheses H1–4 were found to describe the behaviour of transformation trees and forests in this more complex setup well. The loss of using an overly complex model, such as a transformation model with $P = 6$, was tolerable in the simple
normal setups but the gains, especially when parameters of a skewed target depend on the predictor variables, was found to be quite substantial.

7.6. Illustration: Swiss Body Mass Indices

Finally, to conclude this section, we illustrate the applicability of transformation trees and forests in a realistic situation by modelling the conditional body mass index (BMI = weight (in kg) / height (in m)$^2$) distribution for Switzerland, based on 16,427 individuals aged between 18 and 74 years from the 2012 Swiss Health Survey (Bundesamt für Statistik 2013). The predictor variables included smoking, sex, age, and a number of “lifestyle variables” $x$: fruit and vegetable consumption, physical activity, alcohol intake, level of education, nationality and place of residence. Smoking status was categorised into never, former, light, moderate, and heavy smokers. A more detailed description of this data set can be found in Lohse et al. (2017) and extended transformation models for body mass indices are discussed by Hothorn (2018a).

The conditional transformation model underlying transformation trees and transformation forests

$$P(BMI \leq y \mid \text{sex, smoking, age, } x) = F_Z \left( a_{B5,5}(y)^\top \vartheta(\text{sex, smoking, age, } x) \right),$$

assumes that each conditional distribution is parameterised in terms of a Bernstein polynomial with $P = 5$. The parameters $\vartheta$ of this polynomial, however, might depend on the predictor variables in a potentially complex way, featuring interactions and non-linearities. Transformation trees and forest allow such conditional parameter functions $\vartheta$, and thus the corresponding conditional BMI distributions, to be estimated in a black-box manner without the necessity to a priori specify any structure of $\vartheta$ (models assuming such structures are discussed in Hothorn 2018a).

The in-sample negative log-likelihood of the tree presented in Figure 6 is 43079.42. The first split was in sex, so in fact two sex-specific models are given here. Four age groups ($\leq 34, (34, 51], > 51$) for females and three age groups ($\leq 25, (25, 36], > 36$) for males were distinguished. Education contributed to understanding the BMI distribution of females and males. Location, scale and shape of the conditional BMI distributions varied considerably. Higher BMI variability was linked to higher average BMI values. Mean and variance increased with age, and higher-educated people tended to have lower BMI values. These are interesting insights, but this tree model is, of course, very rough.

A transformation forest allows less rough conditional parameter functions $\vartheta$ to be estimated. The negative log-likelihood was 42520.18 and thus a substantial improvement over the negative log-likelihood 43079.42 of the transformation tree. However, such black-box models are rather difficult to understand in terms of the impact of the predictor variables on the conditional BMI distribution. We used a partial dependency plot for conditional deciles to visualise the association between sex, smoking, age and BMI.
as estimated by the transformation forest (Figure 7). In general, the median BMI increases with age, as does the BMI variance. For males, there seemed to be a level-effect whose onset depends on smoking category. Females tended to higher BMI values, and the variance was larger compared to males. There seemed to be a bump in BMI values for females, roughly around 30 years. This corresponds to mothers giving birth to their first child around this age. It is important to note that the right-skewness of the conditional BMI distributions renders conditional normal distributions inappropriate, even under variance heterogeneity.

8. Algorithmic Variants and Their Computational Complexity

The computational complexity of transformation trees and forests basically depends on the variable and split selection performed in every node of the corresponding trees. In this section, we present several possible algorithms for the selection of the “best” binary split and discuss corresponding statistical properties and computational complexities. For a discussion regarding the complexity of random forests we refer to Louppe (2015).

Many prominent tree algorithms, such as CART (Breiman et al. 1984) or C4.5 (Quinlan 1993) evaluate all possible binary splits in all predictor variables via an exhaustive search. For transformation trees, an exhaustive search

$$\hat{B} = \arg \max_{B \subseteq \mathcal{X}} \max_{\vartheta_1, \vartheta_2 \in \Theta} \sum_{i=1}^{N} I(x_i \in B)\ell_i(\vartheta_1) + \sum_{i=1}^{N} I(x_i \notin B)\ell_i(\vartheta_2)$$

would require to evaluate the log-likelihood for all possible splits in $O(PN^2)$. In addition, variable selection based on an exhaustive search would be biased towards variables with many potential splits (Kass 1980). Unbiased recursive partitioning (for example Loh and Shih 1997; Hothorn et al. 2006b; Zeileis et al. 2008) separates variable and split selection to address this bias and to reduce the complexity. Therefore, transformation trees extend the concept of unbiased recursive partitioning by first selecting the most important predictor variable by means of a permutation score test and, in a second step, by finding the best split in this variable as follows (for the sake of simplicity we consider the root node only).

8.1. Variable Selection

Transformation trees select the predictor variable with highest association to the score vector as measured by the $p$-value of a permutation test using the following procedure:

1. Compute the maximum likelihood estimator $\hat{\vartheta}_{\text{ML}}^N$ in $O(PN)$.
2. Compute the score vector $s(\hat{\vartheta}_{\text{ML}}^N \mid Y = y_i) \in \mathbb{R}^P$ for each observation $i = 1, \ldots, N$ in $O(PN)$.
3. For each predictor variable $j = 1, \ldots, J$, compute the linear statistic

$$T_j = \sum_{i=1}^{N} g(x_{ij})s(\hat{\vartheta}_{\text{ML}}^N \mid Y = y_i)^T,$$

where $x_{ij}$ is the value of the $j$-th predictor variable for the $i$-th observation. The time complexity depends on $g$ and the measurement scale of $X_j$. For a simple test with
high power directed towards linear alternatives \( g(x) = x \) is used, with time complexity \( O(PN) \). For a maximally-selected statistic with \( g(x) = I(x < x_{ij}'), i' = 1, \ldots, N \), directing high power towards abrupt-change alternatives, the complexity increases to \( O(PN \log N) \) when the number of potential splits \( x_{ij}' \) is allowed to grow with \( N \).

4. Compute all \( P \) corresponding test statistics

\[
\max \left| \frac{T_j - \mathbb{E}(T_j)}{\text{diag}(\mathbb{V}(T_j))} \right| \quad \text{or} \quad (T_j - \mathbb{E}(T_j))\mathbb{V}(T_j)^{-1}(T_j - \mathbb{E}(T_j))
\]

in \( O(P) \) (best case with \( g(x) = x \)) or \( O(PN) \) (worst case for a maximally selected statistic) and derive the corresponding \( p \)-value in \( O(1) \). \( \mathbb{E}(T_j) \) and \( \mathbb{V}(T_j) \) are the conditional expectation and covariance given all admissible permutations, see Strasser and Weber (1999); Hothorn et al. (2006a). Select the variable with lowest \( p \)-value.

With \( g(x) = x \) transformation trees perform the variable selection in \( O((J + 2)PN) \) instead of the usual \( O(JN \log N) \) when an exhaustive search strategy is employed (for example, in CART). The test statistic has high power (and thus the corresponding predictor variable has a high probability of being selected) when the association to at least one score is linear. In contrast, the test has low power for \( U \)-shaped associations, for example. In such cases, maximally selected statistics with complexity \( O(2PN + JN \log N) \) have a higher power for detecting such patterns.

Thus, adopting such an inference-based variable selection as opposed to exhaustive search may also reduce computational complexity. However, unbiasedness is the more important reason for incorporating the inference-based variable selection from Hothorn et al. (2006b) and Zeileis et al. (2008) into transformation trees.

8.2. Split Selection

Once a predictor variable was selected for splitting, two possible ways for determining the best split exist. Model-based recursive partitioning (Zeileis et al. 2008) maximises the log-likelihood over all possible splits in \( O(N^2) \). Transformation trees follow the approach implemented in conditional inference trees (Hothorn et al. 2006b) and select the split based on the score contributions by a maximally selected statistics of the form

\[
T_{i'} = \sum_{i=1}^{N} I(x_{ij} < x_{i'j})s(\hat{\vartheta}_{\text{ML}}^{N} | Y = y_i)^\top, i' = 1, \ldots, N
\]

in \( O(PN \log N) \). The best split maximises one of the test statistics

\[
\max \left| \frac{T_{i'} - \mathbb{E}(T_{i'})}{\text{diag}(\mathbb{V}(T_{i'}))} \right| \quad \text{or} \quad (T_{i'} - \mathbb{E}(T_{i'}))\mathbb{V}(T_{i'})^{-1}(T_{i'} - \mathbb{E}(T_{i'}))
\]

for the experiments in Section 7 we used the latter quadratic form.

8.3. Empirical Timings

We compared the run times of the algorithms evaluated in Section 7 based on model (7) in the informative low-dimensional setting with varying mean and variance for increasing sample
sizes. In addition, we added versions of transformation trees with exhaustive evaluation of all possible splits in the selected variable by optimising the log-likelihood directly (“exh”). Figure 8 presents the timings in seconds.

[Figure 8 about here.]

CTree and TTree are both based on a linear test statistic with $g(x) = x$ and a split selection via a maximally selected score statistic (9). Because steps (1–4) of the variable selection require most of the time, the total run time is roughly linear in the number of observations $N$. In contrast, when the split is determined by the maximisation of the log-likelihood (the “exh” option), the split selection dominates and the increased complexity is visible in the plot.

Note that while the absolute run times differ between algorithms (evident in the varying y-axis limits), these must not be interpreted as properties of the algorithms. They just reflect different software design decisions: For example, the randomForest package (Breiman et al. 2015) relies on Breiman and Cutler’s original Fortran implementation and is relatively fast but hard to extend or modify. In contrast, the partykit package (Hothorn and Zeileis 2015, 2017) implements a toolbox for recursive partitioning in high-level R code which is slower but very flexible and easy to extend. Therefore, transformation trees and forests required relatively little additional R code (~500 lines) because the infrastructure from partykit and the mlt package for estimating transformation models (Hothorn 2017a,b) were straightforward to reuse.

To check whether trees with and without exhaustive search differ systematically in their predictive performance, Figure 9 presents a comparison of out-of-sample negative log-likelihoods based on model (7). Overall, the performance was roughly the same in this situation indicating that the faster score-based approach was able to identify splits appropriately in this situation. The empirical complexity of all forest variants was roughly the same, mainly because the conceptual forest algorithm employed was the same and the only difference was due to the variable and split selection.

[Figure 9 about here.]

8.4. Potential for Optimisation

One potential source of further optimisation is the ability of transformation models to deal with interval-censored targets. If one bins the targets $y_i$ into $L+1$ bins at breaks $-\infty < y_{(1)} < \cdots < y_{(L)} < \infty$, a model $P_{Y,\theta}$ of higher complexity can be fitted by maximising the weighted log-likelihood for interval-censored observations $\log(F_Z(h(y_{(l)})) - F_Z(h(y_{(l-1)})))$ when $y_{(l-1)} < y_i \leq y_{(l)}$. Evaluation of the likelihood involves now only $K$ instead of $N$ summands when the data were tabulated first. In combination with binned predictor variables, improvements with respect to computing time and memory consumption are possible because the linear statistic $T_j$ can be computed based on the contingency table of the binned target and the binned predictor variable.

9. Discussion

Transformation forests, as well as the underlying transformation trees, can be understood as
adaptive local likelihood estimators in the rather general parametric transformation family of distributions. Owing to possible interactions and non-linear effects in a “black-box” conditional parameter function $\vartheta(x)$, the resulting conditional distributions of the target may depend on the predictors in a very general way. The ability to model the impact of some predictors on the whole conditional distribution simultaneously, including its mean and higher moments, is a unique feature of this novel member of the random forest family. The likelihood approach taken here also directly allows the procedures to be applied to randomly censored or truncated observations.

The algorithmic internals of transformation trees are rooted in conditional inference trees (Hothorn et al. 2006b) and model-based recursive partitioning (Zeileis et al. 2008) and inherit the unbiased variable selection property from these ancestors. Transformation forests also allow for unbiased variable importances (Strobl et al. 2007), including the internal handling of missing predictor variables (Hapfelmeier et al. 2014). An open-source implementation of transformation trees and transformation forests based on the partykit add-on package (Hothorn and Zeileis 2015) to the R system for statistical computing is available as add-on package trtf (Hothorn 2018b), see Appendix “Computational Details”.

Within the theory of adaptive local likelihood estimation, alternative choices for parametric models (via their likelihood contributions $\ell_i(\vartheta)$) and weights $w_i^N(x)$ are possible. In the context of personalised medicine or personalised marketing, one is interested in the dependency of some treatment effect $\beta$ on predictors $x$. Random forest-type algorithms are a promising tool for modelling complex effects of predictors on such a treatment parameter (Foster et al. 2011; Seibold et al. 2016; Wager and Athey 2017; Seibold et al. 2017). In the framework presented here, implementation of such a strategy only requires the specification of a distribution $\mathbb{P}(Y \leq y \mid \text{treated}) = F_Z(a(y)\vartheta + \beta)$ for treated and $\mathbb{P}(Y \leq y \mid \text{untreated}) = F_Z(a(y)^T\vartheta)$ for untreated observations. The model, and therefore also the treatment effect $\beta$, can then be partitioned or aggregated by transformation trees and transformation forests leading to a random forest estimate $\hat{\beta}_N^\text{Forest}(x)$ of the conditional treatment effect $\beta(x)$ in addition to $\hat{\vartheta}_N^\text{Forest}(x)$. Breiman and Cutler’s random forests were empirically shown to be insensitive to changes in treatment effects $\beta$ (in comparison to adaptive local likelihood estimation of very simple parametric models, such as logistic or Weibull regression, Seibold et al. 2017). This corresponds to the empirical findings reported in Section 7 showing an insensitivity of Breiman and Cutler’s random forests to changes in the variance of a conditional normal distribution. Transformation trees and forests, in contrast, were specifically designed to detect such distributional changes by an assessment of parameter stability. This property extends to additional parameters in more complex transformation models featuring predictor-varying effects $\vartheta(x)$ and $\beta(x)$ of the form

$$\mathbb{P}(Y \leq y \mid X = x, U = u) = F_Z(a(y)^T\vartheta(x) + u^T\beta(x))$$

which describe the most general model class associated with transformation trees and forests. Unlike the local normal linear models studied in Bloniarz et al. (2016), the general framework proposed here allows for varying linear effects $\beta(x)$ of additional predictor variables $u$ (as, for example, treatment effects in randomised trials or a priori known confounders in observational studies). Beyond this additional modelling flexibility and unlike Breiman and Cutler’s random forests, transformation trees and forests also allow for all types of target variables under all forms of random censoring or truncation (an overview on known and unknown models from this class is available from Section 4.3 and Table 1 in Hothorn et al. 2017). When parameter
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estimates for such a transformation model are already given (i.e., when some elements of \( \beta(x) \) are available from an external source and shall be kept fix, for example some established treatment effect), one could use transformation forests to estimate a deviation from this initial model. An already existing transformation function can be used as an offset in the likelihood \( \ell_i \), such that the forest conditional parameter function excludes these existing effects.

A more general understanding of weights could be derived from the notion of applying a distance measure \( d \) to two distributions \( \hat{P}_{Y|X=x} = \hat{P}_{Y,\hat{\vartheta}(x)} \) and \( \hat{P}_{Y|X=x_i} = \hat{P}_{Y,\hat{\vartheta}_i(x_i)} \) obtained from the \( t \)-th tree. Based on this distance, an alternative weight could be defined by

\[
\begin{align*}
    w_{Forest,t}^N(x) &= \sum_{t=1}^{T} \left( 1 - d \left( \hat{\vartheta}_{Tree,t}^N(x), \hat{\vartheta}_{Tree,t}^N(x_i) \right) \right)
\end{align*}
\]

for example using the Kullback-Leibler divergence for continuous distributions

\[
d_{KL}(\vartheta_1, \vartheta_2) = \int f_Y(y \mid \vartheta_1) \log \left( \frac{f_Y(y \mid \vartheta_1)}{f_Y(y \mid \vartheta_2)} \right) dy
\]

(after standardisation to the unit interval). This weight takes the conditional distribution in two terminal nodes of a tree into account, rather than just treating them as “somehow different” in the way of nearest neighbour weights.

The empirical evaluation of transformation trees and transformation forests for censored targets (and comparison to a new competitor which is based on splits maximising the integrated absolute difference between conditional survivor curves, recently published by Moradian et al. 2016) as well as the evaluation of the quality of likelihood-based permutation variable importance (including the conditional variable importance) for variable selection, of the model-based bootstrap for variability assessment, and of the likelihood-ratio test are ongoing research projects.

References

Beran R (1988). “Prepivoting Test Statistics: A Bootstrap View of Asymptotic Refinements.” Journal of the American Statistical Association, 83(403), 687–697. doi:10.2307/2289292.

Biau G (2012). “Analysis of a Random Forests Model.” Journal of Machine Learning Research, 13(1), 1063–1095. URL http://jmlr.org/papers/v13/biau12a.html.

Biau G, Devroye L (2010). “On the Layered Nearest Neighbour Estimate, the Bagged Nearest Neighbour Estimate and the Random Forest Method in Regression and Classification.” Journal of Multivariate Analysis, 101(10), 2499–2518. doi:10.1016/j.jmva.2010.06.019.

Biau G, Devroye L, Lugosi G (2008). “Consistency of Random Forests and Other Averaging Classifiers.” Journal of Machine Learning Research, 9, 2015–2033. URL http://jmlr.org/papers/v9/biau08a.html.

Biau G, Scornet E (2016). “A Random Forest Guided Tour.” Test, 25(2), 197–227. doi:10.1007/s11749-016-0481-7.
Bloniarz A, Wu C, Yu B, Talwalkar A (2016). “Supervised Neighborhoods for Distributed Nonparametric Regression.” In “Proceedings of the 19th International Conference on Artificial Intelligence and Statistics,” pp. 1450–1459. URL http://proceedings.mlr.press/v51/bloniarz16.pdf.

Breiman L (2001). “Random Forests.” Machine Learning, 45(1), 5–32. doi:10.1023/A:1010933404324.

Breiman L (2004). “Consistency for a Simple Model of Random Forests.” Technical Report 670, Statistics Department, University of California at Berkeley, California. URL http://www.stat.berkeley.edu/~breiman/RandomForests/consistencyRFA.pdf.

Breiman L, Cutler A, Liaw A, Wiener M (2015). Breiman and Cutler’s Random Forests for Classification and Regression. R package version 4.6-12, URL https://CRAN.R-project.org/package=randomForest.

Breiman L, Friedman JH, Olshen RA, Stone CJ (1984). Classification and Regression Trees. Wadsworth, California.

Brillinger DR (1977). “Discussion of Stone (1977).” The Annals of Statistics, 5(4), 622–623.

Bundesamt für Statistik (2013). Die Schweizerische Gesundheitsbefragung 2012 in Kürze – Konzept, Methode, Durchführung. Bern. URL http://www.bfs.admin.ch.

Criminisi A, Shotton J, Konukoglu E (2012). “Decision Forests: A Unified Framework for Classification, Regression, Density Estimation, Manifold Learning and Semi-Supervised Learning.” Foundations and Trends in Computer Graphics and Vision, 7(2–3), 81–227. doi:10.1561/0600000035.

Curtis SM, Ghosh SK (2011). “A Variable Selection Approach to Monotonic Regression with Bernstein Polynomials.” Journal of Applied Statistics, 38(5), 961–976. doi:10.1080/02664761003692423.

Efron B, Tibshirani RJ (1993). An Introduction to the Bootstrap. Chapman & Hall, New York.

Farouki RT (2012). “The Bernstein Polynomial Basis: A Centennial Retrospective.” Computer Aided Geometric Design, 29(6), 379–419. doi:10.1016/j.cagd.2012.03.001.

Foster JC, Taylor JM, Ruberg SJ (2011). “Subgroup Identification from Randomized Clinical Trial Data.” Statistics in Medicine, 30(24), 2867–2880. doi:10.1002/sim.4322.

Friedman JH (1991). “Multivariate Adaptive Regression Splines.” The Annals of Statistics, 19(1), 1–67.

Gneiting T, Balabdaoui F, Raftery AE (2007). “Probabilistic Forecasts, Calibration and Sharpness.” Journal of the Royal Statistical Society B, 69(2), 243–268. doi:10.1111/j.1467-9868.2007.00587.x.

Gneiting T, Raftery AE (2007). “Strictly Proper Scoring Rules, Prediction, and Estimation.” Journal of the American Statistical Association, 102(477), 359–378. doi:10.1198/016214506000001437.
Hapfelmeier A, Hothorn T, Ulm K, Strobl C (2014). “A New Variable Importance Measure for Random Forests with Missing Data.” *Statistics and Computing*, **24**(1), 21–34. doi:10.1007/s11222-012-9349-1.

Hothorn T (2017a). *mlt: Most Likely Transformations*. R package version 0.2-2, URL http://CRAN.R-project.org/package=mlt.

Hothorn T (2017b). *Most Likely Transformations: The mlt Package*. R package vignette version 0.2-1, URL https://CRAN.R-project.org/package=mlt.docreg.

Hothorn T (2018a). “Top-Down Transformation Choice.” *Statistical Modelling*. URL https://arxiv.org/abs/1706.08269.

Hothorn T (2018b). *Transformation Trees and Forests*. R package version 0.3-0, URL https://CRAN.R-project.org/package=trtf.

Hothorn T, Hornik K, van de Wiel MA, Zeileis A (2006a). “A Lego System for Conditional Inference.” *The American Statistician*, **60**(3), 257–263. doi:10.1198/000313006X118430.

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

Hothorn T, Kneib T, Bühlmann P (2014). “Conditional Transformation Models.” *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **76**(1), 3–27. doi:10.1111/rssb.12017.

Hothorn T, Lausen B, Benner A, Radespiel-Tröger M (2004). “Bagging Survival Trees.” *Statistics in Medicine*, **23**(1), 77–91. doi:10.1002/sim.1593.

Hothorn T, Möst L, Bühlmann P (2017). “Most Likely Transformations.” *Scandinavian Journal of Statistics*. doi:10.1111/sjos.12291.

Hothorn T, Zeileis A (2015). “partykit: A Modular Toolkit for Recursive Partytioning in R.” *Journal of Machine Learning Research*, **16**, 3905–3909. URL http://jmlr.org/papers/v16/hothorn15a.html.

Hothorn T, Zeileis A (2017). *partykit: A Toolkit for Recursive Partitioning*. R package version 1.2-0, URL https://CRAN.R-project.org/package=partykit.

Ishwaran H, Kogalur UB, Blackstone EH, Lauer MS (2008). “Random Survival Forests.” *The Annals of Applied Statistics*, **2**(3), 841–860. doi:10.1214/08-aoas169.

Kass GV (1980). “An Exploratory Technique for Investigating Large Quantities of Categorical Data.” *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, **29**(2), 119–127. doi:10.2307/2986296.

Lin Y, Jeon Y (2006). “Random Forests and Adaptive Nearest Neighbors.” *Journal of the American Statistical Association*, **101**(474), 578–590. doi:10.1198/016214505000001230.

Lindsey JK (1996). *Parametric Statistical Inference*. Clarendon Press, Oxford.
Loader C (1999). *Local Regression and Likelihood*. Springer-Verlag, New York.

Loh WY, Shih YS (1997). “Split Selection Methods for Classification Trees.” *Statistica Sinica*, 7, 815–840.

Lohse T, Rohrmann S, Faeh D, Hothorn T (2017). “Continuous Outcome Logistic Regression for Analyzing Body Mass Index Distributions.” *F1000Research*, 6, 1933. doi:10.12688/f1000research.12934.1.

Louppe G (2015). “Understanding Random Forests: From Theory to Practice.” Technical report, arXiv 1407.7502, v3. URL http://arxiv.org/abs/1510.04342.

Mayr A, Hothorn T, Fenske N (2012). “Prediction Intervals for Future BMI Values of Individual Children–A Non-Parametric Approach by Quantile Boosting.” *BMC Medical Research Methodology*, 12, 6. doi:10.1186/1471-2288-12-6.

Meinshausen N (2006). “Quantile Regression Forests.” *Journal of Machine Learning Research*, 7, 983–999. URL http://jmlr.org/papers/v7/meinshausen06a.html.

Meinshausen N (2017). quantregForest: Quantile Regression Forests. R package version 1.3-7, URL https://CRAN.R-project.org/package=quantregForest.

Moradian H, Larocque D, Bellavance F (2016). “$L_1$ Splitting Rules in Survival Forests.” *Lifetime Data Analysis*. doi:10.1007/s10985-016-9372-1.

Quinlan RR (1993). *C4.5: Programs for Machine Learning*. Morgan Kaufmann Publishers, San Francisco, California.

R Core Team (2016). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. URL https://www.R-project.org/.

Scornet E, Biau G, Vert JP (2015). “Consistency of Random Forests.” *The Annals of Statistics*, 43(4), 1716–1741. doi:10.1214/15-AOS1321.

Seibold H, Zeileis A, Hothorn T (2016). “Model-Based Recursive Partitioning for Subgroup Analyses.” *International Journal of Biostatistics*, 12(1), 45–63. doi:10.1515/ijb-2015-0032.

Seibold H, Zeileis A, Hothorn T (2017). “Individual Treatment Effect Prediction for ALS Patients.” *Statistical Methods in Medical Research*. doi:10.1177/0962280217693034.

Stone CJ (1977). “Consistent Nonparametric Regression (with Discussion).” *The Annals of Statistics*, 5(4), 595–645. doi:10.1214/aos/1176343886.

Strasser H, Weber C (1999). “On the Asymptotic Theory of Permutation Statistics.” *Mathematical Methods of Statistics*, 8, 220–250. Preprint available from http://epub.wu-wien.ac.at/dyn/openURL?id=oai:epub.wu-wien.ac.at:epub-wu-01_94c.
Appendix

Computational Details

A reference implementation of transformation trees and transformation forests is available in the `trtf` package (Hothorn 2018b). This package was built on top of the infrastructure packages `partykit` (Hothorn and Zeileis 2015, 2017) and `mlt` (Hothorn 2017a,b). Conditional inference trees and forests were fitted using package `partykit`. Quantile regression forests were computed by the `quantregForest` package (Meinshausen 2017). The reference implementation of Breiman’s and Cutler’s random forests in the `randomForest` package (Breiman et al. 2015) was used. All computations were performed using R version 3.4.3 (R Core Team 2016).

For the empirical evaluation in Section 7, all non-linear transformation models were based on transformation functions parameterised in terms of Bernstein polynomials of order five, i.e., with six parameters, and $F_Z = \Phi$. Log-likelihoods were optimised under monotonicity constraints using a combination of augmented Lagrangian minimisation and spectral projected gradients. Unbiased trees, including transformation trees, stopped internally when the minimum Bonferroni-adjusted $p$-value was larger than 0.05. No such internal stopping was applied in conditional inference or transformation forests. Subsampling of $0.632N$ observations was used for all random forest-types. The minimum number of observations necessary for splitting (`minsplit` in `partykit` and `nodesize` in `randomForest`) was 25 for all forest types in the simulation experiments.

Data from the Swiss Health Survey 2012 can be obtained from the Swiss Federal Statistics Office (Email: sgb12@bfs.admin.ch). Data is available for scientific research projects, and a data protection application form must be submitted. More information can be found here http://www.bfs.admin.ch/bfs/de/home/statistiken/gesundheit/erhebungenSupplementary. The code used for producing the results for the body mass illustration can be evaluated on a smaller artificial data set sampled from the transformation forest by running `demo("BMI")`
from the \texttt{trtf} package (Hothorn 2018b); Figure 1 is regenerated by \texttt{demo("QRF")}. The simulation results presented in this paper can be reproduced using the files in \texttt{system.file("sim", package = "trtf")}.

Additional Results: Empirical Evaluation

Additional Evaluation of Tree-Structured Conditional Parameter Function ($H1a$)

[Figure 10 about here.]

[Figure 11 about here.]

[Figure 12 about here.]

[Figure 13 about here.]

[Figure 14 about here.]

[Figure 15 about here.]

Additional Evaluation of Non-Linear Conditional Parameter Function ($H1b$)

[Figure 16 about here.]

[Figure 17 about here.]

[Figure 18 about here.]

[Figure 19 about here.]

[Figure 20 about here.]

[Figure 21 about here.]

Review History: Version 1 by Journal 1 (January 2017–May 2017)

Review for version 1 (https://arxiv.org/abs/1701.02110v1). Comments by referees are printed in \textit{italics}, replies by the authors in plain text.

Handling Editor

Both reports find the paper interesting in that it combines partitioning methods with local likelihood estimation. However, they also raise very good questions about the paper. I have also taken a look at the paper myself. I highlight the important points/issues below, combining the reports’ comments and my own:
Transformation Forests

1. **Computational complexity of the proposed method, especially in high-dimension, needs to be addressed.**

We added a new Section 8 containing a detailed description of the variable and split selection methods in transformation trees. This section also discusses the statistical properties and the computational complexity of these variants. The theoretical findings are supported by an analysis of the empirical runtimes.

2. **Reproducibility of the experimental results is unclear. That is, the simulation set-ups are not clear enough for a reader to reproduce the results by writing their own codes. Please make the results reproducible.**

GPL-2 licensed open-source code implementing transformation trees and forests is available from CRAN since 2018-01-08 (package `trtf`). The revision now contains a link to the source code for the artificial simulation experiments. Reproducibility material for the body weight application is published with Hothorn (2018). These issues are discussed in Section “Computational Details”.

3. **A much clearer description is needed on how your proposed method is built on existing works in the literature, and please cite all appropriate papers (the second report mentions a few more).**

We agree that the description of unbiased model-based recursive partitioning was a little too opaque in the first version. We comment on statistics used for variable and split selection in unbiased model-based recursive partitioning (and thus also by transformation trees) now in much more detail in our new Section 8.

4. **More explanation and evidence on why a new method like yours is needed too, given the many related method – I understand that interpretability is a motivation, did you illustrate clearly the interpretability of your new method in the data example?**

We believe that the new simulation experiments support our main hypothesis that none of the existing tree or forest algorithms is able to detect distributional changes unrelated to the mean. Transformation trees and forests fill this gap. This fact is prominently stated in the introduction and throughout the manuscript and motivated the design of the new simulation experiments. The new illustration regarding body weight gives an (as we hope) easy to understand impression of how transformation trees and forests detect and represent distributional changes in higher moments of the conditional distribution of the target given predictor variables.

5. **Computational complexity comparisons to representatives of the existing methods, including in terms of running times of your method and others in the experimental results section.**

See point 1.

6. **Since RF is commonly used in practice rather than the model-based partitioning method, it is necessary to use one version of RF, for example, the one by Breiman, in place of the model-based partitioning method, to generate weights used in the proposed method. Comparisons to this RF-based version of the proposed methods in terms of computational complexity (running time) and prediction and confidence interval metrics are needed.**
We agree that most readers will be interested in a direct comparison with Breiman and Cutler’s randomForests. The new simulation experiments directly compare transformation trees and forests as well as conditional inference trees and forests with this reference implementation of random forests. We followed the suggestion to estimate a conditional transformation model based on weights extracted from Breiman and Cutler’s randomForests. Therefore, a direct comparison to transformation forests on the same scale is now presented. Prediction error is assessed based on the out-of-sample log-likelihood and prediction intervals are evaluated based on the 10% and 90% check risk. Theoretical and empirical runtimes are studied in our new Section 8.

7. Moreover, I am not convinced that model-based bootstrap is a good method to use for uncertainty measures, especially in high-dim and when the data generating model is misspecified or is a mis-match for the parametric models used in your method.

We did not evaluate the quality of the model-based bootstrap (Section 5.3) nor size and power of the likelihood-ratio test (Section 5.4) in the initial submission. The main point we were trying to make in Section 5 was that the understanding of transformation forests as parametric models allows such procedures to be implemented. The model-based bootstrap for the approximation of the null distribution of likelihood-ratio statistics was introduced already in the late 1980ies (two references were added). Its size of course depends on how well the null model describes the data and how much the transformation forest overfits the data. We investigate the latter issue in the new artificial simulation experiments in Section 7, also in the presence of non-informative predictor variables. We now explicitly mention (in the discussion) that an empirical evaluation of likelihood-based variable importances for variable selection, the model-based bootstrap for variability assessment and of the likelihood-ratio test are ongoing research projects.

Reviewer 1

1. Your general framework is very clear, it is a good idea, and it fits very well into results which already exist about random forest.

   Thank you!

2. You are splitting the space in such a way that the second expression on page 8 is maximized.

   We regret the confusion caused by the second formula on page 8, which suggested that an exhaustive search is performed. Unbiased recursive partitioning avoids exhaustive evaluations of all potential splits by a separation of variable and split selection. The formula was understood as an illustration of the concept, not the actual implementation. We moved this formula to Section 8 and added a much more detailed description of variable and split selection in transformation trees.

   If I understand that correctly, then you approximate the true likelihood by the “exact continuous” approximation instead of the correct likelihood function as on page 6. I can see that this can make sense when the partitions are very small. But isn’t that a problem in the beginning when the partition is very big or in high dimensions? Is there
a computational reason for doing this? Have you done simulations, how that choice affects the performance of your estimator?

We are sorry for the insufficient description of the different likelihood contributions. The “approximation” of the “exact” likelihood by the density is a rather uncommon (at least outside survival analysis) concept. However, the theory of transformation models is closely tied to the understanding and evaluation of the “exact” likelihood for interval-censored observations. Because we can never observe real numbers (only intervals), we felt it would help to think of the “exact” likelihood as a probability (the definition by Fisher dating back to 1922 in fact advocates this point of view). We rephrased this paragraph and separately introduce the likelihood for real numbers and intervals now. The new Section 8 also introduces a potential application of the interval-censored likelihood as a means for reducing runtimes of the algorithm.

3. In general, I wonder to what extend the argmax on page 8 is realizable? That seems quite costly to me. The best split in random forest can be found in $O(p \times n \times \log(n))$. How does this expression compare, if you only consider axis-aligned slits of $p$ features with $n$ possible splitting points? It would be nice to see an expression of the computational complexity and a runtime comparison in terms of $n$ and $p$.

You are right, of course. We discuss theoretical and empirical runtimes in more detail in our new Section 8.

4. Furthermore, the score function is used as a pruning criteria which totally makes sense for single regression trees, but in the standard Random Forest, people usually do not do such pruning. Have you considered not to implement this pruning criterion? One could perform splits until at least $k$ observations are left in each leaf. Wouldn’t that speed up the simulation? Your random forest version could perform better.

We apologise for not being more precise in the description of our implementation of transformation forests. Of course, forests aggregate over trees built without internal stopping. For transformation trees it makes sense to restrict terminal nodes to a certain number of observations because it won’t be possible to estimate the parameters of the transformation model (and thus to compute the score matrix) with $N$ being too small. Because the size of a terminal node cannot be controlled directly in the randomForest package (the parameter nodesize corresponds to minsplit but not minbucket in rpart or partykit terminology), we required at least 25 observations in order to implement a split for all forest variants under test.

5. For the parametric bootstrap, why would you throw away those “extreme” samples? That can make sense, but throwing them away would not be the parametric bootstrap, and there is some intuition which I might be missing.

You are right, the distribution of the likelihood ratio statistic is not the only bootstrap distribution one could be interested in. We replaced this paragraph explaining that one can look at the bootstrap distribution of the parameters $\vartheta(x)$ or any functional thereof (including the LR statistic).

6. I wonder whether this is the right Likelihood-Ratio Test. What if the true distribution is independent of $X$, but it is very complicated and cannot be approximated by your unconditional maximum likelihood model. Then your original statistics has a completely
Of course. We clarified (in Section 2, see also point “p.6, l.-4” by referee 2) that we assume that the true transformation function can be written as $h = a^\top \vartheta$ throughout the manuscript. Under this condition, the procedure is just the simple parametric bootstrap. See also point 7 by the editor.

7. Furthermore, it would also be nice to have an intuitive statement of how the choice of the set in which $h$ lies affects the bias-variance trade-off.

We explicitly cover this point in the empirical evaluations in Section 7 now. The empirical effects of using the ‘correct’ transformation function (for example, a linear function for conditionally normal targets) compared to an overparameterised (ie, non-linear) version are investigated in a simulation model with normal targets. For log-normal targets, the loss of using an underparameterised (linear) transformation function is also presented.

8. The way I understand your simulation setup is the following: You take real data sets, you fit each method, and then you use the parametric bootstrap to create from each fitted estimator new data sets. Those new data sets have the same feature points but $Y$ values created from the fitted models. To compare with fully non-parametric estimators (such as quantile regression forest) wouldn’t it make more sense to use a bigger data set, use on one part of it as a training data set and use the rest as an evaluation data set? At least for confidence intervals comparisons that would be very appealing to me and it would be fair since all of your models are essentially based on transformation models, right? If you need access to the true underlying data generating process, it might be worthwhile also comparing your methods to made up data generating processes. Otherwise, you are comparing four estimators with QRF by creating data directly coming from models which are generated by those estimators.

Our intention was to evaluate the methods based on “realistic” simulation models related to a specific algorithm. We think that our comparison with quantile regression forests were correct, because we also directly sampled (nonparametrically) from this model. The main problem with a bootstrap-based simulation is that the “simulation model” is a tree or a forest and only the former can be visualised and directly understood. We also understand the points you and the other reviewer raised and therefore implemented a more traditional simulation study based on artificial data generating processes with separate learning and validation sets in Section 7.

9. There is also an estimator called Density Forest and Manifold Forest, which were for example mentioned in Criminisi et al. 2011. It would be nice to have a comparison to those methods as well.

Thank you very much for pointing us to this interesting publication. Our understanding of http://dx.doi.org/10.1561/0600000035 (page 134) is that the model is conditional normal with predictor-dependent mean and variance. However, it is unclear (in this and other publications from the group) how the underlying trees handle variance heterogeneity that can be explained by the predictor variables (no details regarding the “weak learner” are presented on page 137). The more flexible (as it seems) density and manifold forests are for the unsupervised case only.
The authors provide software for reproducing results presented in a follow-up book (“Sherwood” from https://www.microsoft.com/en-us/download/details.aspx?id=52340&751be11f-ede8-5a0c-058c-2ee190a24fa6=True).

We generated an example data set (Figure 22) and tried to run the software on this example using

./sw regression /t 100 /d 10 th.txt

and obtained the following output

Training the forest...
Trained 100 trees.

Applying the forest to test data...
Applied 100 trees.
Segmentation fault (core dumped)

It also seems that the only output the software can produce is a bitmap file with the original data overlayed with the model. We did not find any possibility to specify test data, let alone a means to compute out-of-sample prediction errors etc. For these reasons it was not possible for us to include this implementation as an additional competitor in the empirical evaluations in Section 7. However, the method is interesting because mean aggregation of conditional densities is performed, and this is similar to the mean aggregation of cumulative hazard functions in random survival forests. The introduction now highlights this similarity.

10. For you confidence interval simulations, there are two things to consider. They should have the correct coverage, and they should be small. I would also be curious how your confidence intervals differ in size.

It is in general hard to compare prediction intervals, because they condition on a specific set of predictor variables. Thus, coverage and lengths can differ substantially over the sample space. We elaborate on this issue in Section 7 and also point to the proper scoring rules literature. However, the check risk for the 10% and 90% quantiles is appropriate to compare the ability of methods to estimate these conditional quantiles and we, in addition to the negative log-likelihood and the absolute error, report these two performance measures.

Little typos: (omitted). Thank you, we silently corrected the typos.

Reviewer 2
Overview  This is an interesting paper. Hothorn and Zeileis describe using weights, say $w_i$ derived from a random forest algorithm to fit the model:

$$\hat{\vartheta}^N(x) := \arg\max_{\vartheta \in \Theta} \sum_{i=1}^{N} w_i^N(x) \ell_i(\vartheta).$$

(10)

The likelihoods are chosen from a transformation family: $F_Y(y) = F_Z(h(y))$ Here $F_Z$ is known a priori (for example it might be the standard Gaussian distribution function) and $h$ is the quantity maximized. Some structure is imposed on $h$ to make the maximization easier. In the examples considered $h$ was modelled by Bernstein polynomials.

Major comments  We suggest that implementing one and only one of the major comments addressed below would make this a very strong paper.

Thank you for the suggestion, we chose the second option.

2.1. Developing directly relevant theoretical results. The authors cite the prior work of Hothorn, Kneib and Bühlmann showing consistency results for conditional transformation forests and it seems straightforward to extend these results to the case where the tree partition is not estimated from the data. They go on to cite recent theoretical work including Scornet at al (2015) that establishes consistency results for an algorithm that is almost the same as Breiman’s original random forests. They suggest that these results can be adapted to show consistent estimation of the likelihood function they seek to maximize. However the development seems slightly heuristic and it would seem that some conditions on the complexity of the likelihood family is required but no conditions are given. Moreover, this is not quite the flavour of theoretical results that are directly relevant. We want a result that says that transformation forests consistently estimate the distribution of $Y \mid X$, where convergence is measured in, for example, KS distance. This is a stronger result than they develop because if, for example, the family of functions chosen to model $h$ does not include the true $h$ then consistent estimation of the likelihood need not imply consistent estimation of $Y \mid X$.

We agree that such results would be extremely important and valuable. Prior to submitting the initial version of this manuscript, we discussed the possibility to obtain such results with Nicolai Meinshausen. The outcome of the discussion was that this task is a major research project in its own right and we therefore refrained from digging deeper here. In addition, our understanding of the theoretical literature on random forests is that practically relevant results (ie, the analysis of non-idealised versions of random forests) are very rare and technically challenging. The main difference between Breiman and Cutler’s randomForests and the transformation forests proposed in this manuscript is with respect to the variable and split selection. We are not aware of a paper analysing the impact of different forms of variable and split selection on the theoretical performance of random forests.

2.2. Providing richer simulations covering high dimensional settings. Alternatively if theoretical results are unduly difficult it would be worthwhile to provide a richer set of simulations. All datasets from which the simulations are derived have $N \leq 4177$ and $p \leq 18$; the maximal aspect ratio of the data is 16.9. These simulation settings appear to be derived from Meinshausen’s quantile forests paper. None of these settings are
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especially relevant for high dimensional problems, where Breiman’s random forest has been especially successful. While it is certainly true that distribution estimation requires much more data than the estimation of the conditional mean it seems worthwhile to at least investigate the performance of transformation forests in high dimensional settings.

We agree with your criticism and the criticism raised by reviewer 1 (see 8 by reviewer 1). In the novel simulations based on artificial data generating processes we study the performance of all methods in the low-dimensional situation and the situation with 50 noise variables added.

Minor comments

p.2, l.15 The use of random survival forests is preceded by the paper “Tree structured survival analysis” (1985) by Gordon and Olshen and arguably should be cited, although, because it predates the random forest algorithm, they adapt trees rather than forests.

You are right, of course. In this paragraph, we focus on existing random forest methods for the estimation of conditional distribution (or survivor) functions. We incorrectly cited random survival forests here, because aggregation takes place by averaging cumulative hazard functions (their formula 3.2), so this reference was removed.

p.2, l.16 Lin and Jeon (2006) certainly develop “adaptive nearest neighbours” but it is not obvious to me that they propose they be used for conditional distribution estimation as stated.

Yes, they exclusively focus on conditional means. We highlight this fact now prominently.

p.6, l.12 The fact that $F_Z(\infty) = 1$ and $F_Z(-\infty) = 0$ is implied by the fact that $F_Z$ is a distribution function and should not be stated.

Sorry, a copy-and-paste error from the (more general) description in http://dx.doi.org/10.1111/sjos.12291. Fixed.

p.6, l.16 Often the minimum extreme value distribution is parameterized by the mean and variance to which the minimum value corresponds; consider calling it the standard minimum extreme value distribution.

Thank you, fixed.

p.6, l.-8 “relatively precise measurements”. You seem just to need that the density be relatively constant within an interval; the interval need not be too short.

See 2 by Referee 1.

p.6, l.-4 You parameterize $h$ to “simplify estimation”. I think this is required for more reasons than simplicity. If $h$ were allowed to be any function then there would be no hope of estimating it.

You are right. Throughout the manuscript we assume that the true unknown transformation function can be written in terms of such a basis function. We clarified this fact.
Unbiasedness seems to be used in the sense that variables with more classes are not preferred for splits in the null model of no effect. This is not quite obvious from the context so a sentence clarifying the use of the term would be helpful.

We added a more elaborate description of the variable and split selection procedure, including a discussion of “unbiasedness”, to our new Section 8.

Permutation variable importance is used for random forests despite its many drawbacks because better alternatives are harder to come by. (For example if two features are equal but highly correlated with $Y$ they will seem to have zero importance by this measure). Given the richer parametric structure your estimating it would be nice if a more satisfying measure of variable importance were available.

We agree that permutation variable importance is not an ideal tool for variable selection. We elaborate on the possibility of a conditional variable importance in the revision and state that more empirical insight into the variable selection properties are necessary. We are not convinced that the parametric structure gives us more leverage, because “only” the conditional parameter functions $\vartheta(x)$, i.e., random forest-type black-box functions, determine variable importance in transformation forests.

Can you provide any theoretical guarantees for the model based bootstrap? Typically in low dimensions guarantees are not too difficult to obtain. It would also be deduce whether it fails in high dimensions but this may be quite arduous.

We added (in Section 7) some empirical evidence on the overfitting behaviour of transformation forests. It seems that the amount of overfitting, especially under the null of no association between predictors and target, seems tolerable, indicating that the likelihood-ratio test and also the model-based bootstrap might perform appropriately. However, we did not yet perform tailored experiments on these questions (and explicitly point the reader to ongoing research on these topics in the discussion).

Consider also citing Breiman (2004) “Consistency for a simple model of random forests”. This is the earliest argument of which I know for the consistency of random forests.

Thank you!

Consider citing “Piecewise-polynomial regression trees” (1994).

SUPPORT is one of the earlier references for fitting model-based trees. We reviewed these predecessors of model-based recursive partitioning in Zeileis, Hothorn and Hornik (2008) and refer to this review instead.

Consider citing “Supervised neighborhood for distributed nonparametric regression” by Adam Bloniarz, Christopher Wu, Bin Yu and Ameet Talwalkar (2016). They exploit the neighborhood of Lin and Jeon (2006) in a similar fashion but for a different purpose.

Thank you for pointing us to this relevant paper on local linear model estimation. The paper is now cited in the Introduction and Section 2.
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Figure 1: Empirical Illustration. Conditional on a uniform predictor $x$, the distribution $Y \sim N(0, (1+I(x > .5))^2)$ features a variance split at .5 for 10,000 observations (points outside the conditional 10% and 90% quantile are in red). The black solid line depicts estimated conditional 10% and 90% quantiles obtained from quantile regression forests, the blue lines correspond to quantiles estimated by transformation trees (dashed) and transformation forests (solid) with non-linear transformation function parameterised via a Bernstein polynomial of order five.
Figure 2: Simulation Model (5). Negative log-likelihood differences for trees and forests in a conditional normal model with potential jumps in mean and variance. The negative log-likelihood difference was computed as the out-of-sample negative log-likelihood of each competitor minus the negative log-likelihood of the true data generating process. Outliers were not plotted.
Figure 3: Simulation Model (6). Negative log-likelihood differences for trees and forests in a conditional log-normal model with potential jumps in mean and variance. The negative log-likelihood difference was computed as the out-of-sample negative log-likelihood of each competitor minus by the negative log-likelihood of the true data generating process. Values larger than two were not plotted.
Figure 4: Simulation Model (7). Negative log-likelihood differences for trees and forests in a conditional normal model with non-linear functions defining mean and variance. The negative log-likelihood difference was computed as the out-of-sample negative log-likelihood of each competitor minus the negative log-likelihood of the true data generating process. Outliers were not plotted.
Figure 5: Simulation Model (8). Negative log-likelihood differences for trees and forests in a conditional log-normal model with non-linear functions defining mean and variance. The negative log-likelihood difference was computed as the out-of-sample negative log-likelihood of each competitor minus the negative log-likelihood of the true data generating process. Values larger than two were not plotted.
Figure 6: Body Mass Index (BMI). The conditional BMI distributions (depicted in terms of their densities) are given in each subgroup of the transformation tree (featuring a non-linear transformation function) corresponding to the terminal nodes of the tree. Variables: education (edu) at levels mandatory (I), secondary (II) and tertiary (III); alcohol intake (agramtag).
Figure 7: Body Mass Index (BMI). Partial dependency plot of conditional deciles estimated by a transformation forest with non-linear transformation function.
Figure 8: Empirical Timings. Run times (in seconds) of all methods compared in Section 7 for simulation model (7). Transformation trees with linear ($P = 2$) and non-linear ($P = 6$) transformation function and with score-based split selection (9) and direct maximisation of the log-likelihood (exh) and corresponding forest variants are given.
Figure 9: Simulation Model (7). Log-likelihood ratios for trees and forests in a conditional normal model with non-linear functions defining mean and variance. Transformation trees with linear ($P = 2$) and non-linear ($P = 6$) transformation function and with score-based split selection (9) and direct maximisation of the log-likelihood (exh) are given. Outliers were not plotted.
Figure 10: Simulation Model (5). 10% quantile risk differences for trees and forests in a conditional normal model with non-linear functions defining mean and variance. The quantile risk difference was computed as the out-of-sample check risk of each competitor minus the check risk of the true data generating process.
Figure 11: Simulation Model (5): Absolute error differences for trees and forests in a conditional normal model with non-linear functions defining mean and variance. The absolute error difference was computed as the absolute error of each competitor minus the absolute error of the true data generating process.
Figure 12: Simulation Model (5): 90\% quantile risk differences for trees and forests in a conditional normal model with non-linear functions defining mean and variance. The quantile risk difference was computed as the out-of-sample check risk of each competitor minus the check risk of the true data generating process.
Figure 13: Simulation Model (6). 10% quantile risk differences for trees and forests in a conditional log-normal model with non-linear functions defining mean and variance. The quantile risk difference was computed as the out-of-sample check risk of each competitor minus the check risk of the true data generating process.
Figure 14: Simulation Model (6): Absolute error differences for trees and forests in a conditional log-normal model with non-linear functions defining mean and variance. The absolute error difference was computed as the absolute error of each competitor minus the absolute error of the true data generating process.
Figure 15: Simulation Model (6): 90% quantile risk differences for trees and forests in a conditional log-normal model with non-linear functions defining mean and variance. The quantile risk difference was computed as the out-of-sample check risk of each competitor minus the check risk of the true data generating process.
Figure 16: Simulation Model (7). 10% quantile risk differences for trees and forests in a conditional normal model with non-linear functions defining mean and variance. The quantile risk difference was computed as the out-of-sample check risk of each competitor minus the check risk of the true data generating process.
Figure 17: Simulation Model (7): Absolute error differences for trees and forests in a conditional normal model with non-linear functions defining mean and variance. The absolute error difference was computed as the absolute error of each competitor minus the absolute error of the true data generating process.
Figure 18: Simulation Model (7): 90% quantile risk differences for trees and forests in a conditional normal model with non-linear functions defining mean and variance. The quantile risk difference was computed as the out-of-sample check risk of each competitor minus the check risk of the true data generating process.
Figure 19: Simulation Model (8). 10% quantile risk differences for trees and forests in a conditional log-normal model with non-linear functions defining mean and variance. The quantile risk difference was computed as the out-of-sample check risk of each competitor minus the check risk of the true data generating process.
Figure 20: Simulation Model (8): Absolute error differences for trees and forests in a conditional log-normal model with non-linear functions defining mean and variance. The absolute error difference was computed as the absolute error of each competitor minus the absolute error of the true data generating process.
Figure 21: Simulation Model (8): 90% quantile risk differences for trees and forests in a conditional log-normal model with non-linear functions defining mean and variance. The quantile risk difference was computed as the out-of-sample check risk of each competitor minus the check risk of the true data generating process.
> set.seed(290875)
> N <- 1000
> x <- runif(N, min = -1, max = 1)
> y <- rnorm(N, mean = sin(2 * x * pi), sd = exp(x))
> plot(y ~ x)
> write.table(data.frame(x = x, y = y), file = "th.txt",
+  col.names = FALSE, row.names = FALSE, sep = "\t")

Figure 22: Example to be used for “Sherwood” example code.
Table 1: Competitor Overview. All competitors ordered with respect to variable and split selection procedures as well as complexity of the underlying transformation function $h$. Abbreviations: Mean-squared error (MSE), residual sum of squares (RSS), exhaustive (exh).