Regression Trees for Longitudinal and Clustered Data Based on Mixed Effects Models: Methods, Applications, and Extensions

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Outline of talk

Longitudinal data

Panel or longitudinal data, in which we observe many individuals over multiple periods, offers a particularly rich opportunity for understanding and prediction, as we observe the different paths that a variable might take across individuals. Such data, often on a large scale, are seen in many applications:

- test scores of students over time
- blood levels of patients over time
- transactions by individual customers over time
- tracking of purchases of individual products over time

Longitudinal data

The analysis of longitudinal data is especially rewarding with large amounts of data, as this allows the fitting of complex or highly structured functional forms to the data.

We observe a panel of *individuals* $i = 1, ..., I$ at times $t = 1, ..., T_i$. A single observation period for an individual (i, t) is termed an *observation*; for each observation, we observe a vector of covariates, $\mathbf{x}_{it} = (x_{it1}, ..., x_{itK})'$, and a response, y_{it}.

Longitudinal data models

Because we observe each individual multiple times, we may find that the individuals differ in systematic ways; e.g., y may tend to be higher for all observation periods for individual i than for other individuals with the same covariate values because of characteristics of that individual that do not depend on the covariates. This pattern can be represented by an "effect" specific to each individual (for example, an individual-specific intercept) that shifts all predicted values for individual i up by a fixed amount.

$$y_{it} = Z_{it}\mathbf{b}_i + f(x_{it1}, ..., x_{itK}) + \varepsilon_{it}$$

Fixed and random effects

- If f is linear in the parameters and the b_i are taken as fixed or potentially correlated with the predictors, then this is a linear *fixed effects model* (analysis of covariance).
- If f is linear in the parameters and the b_i are assumed to be random and uncorrelated with the predictors, then the model is a linear *mixed effects model* (with random effects $\mathbf{b}_i$).

Conceptually, random effects are appropriate when the observed set of individuals can be viewed as a sample from a large population of individuals, while fixed effects are appropriate when the observed set of individuals represents the only ones about which there is interest.

Why random effects versus fixed effects?

Random effects models also have some practical advantages over fixed effects models, particularly for large data sets.

- When appropriate, they are more efficient than fixed effects models (especially when T_i is small and I is large), because the number of parameters estimated in a fixed effects model increases with the addition of more individuals.
- Fixed effects models with individual-specific intercepts do not allow the inclusion of predictors that are always constant for individuals, such as gender (when individuals are people) or product type (when individuals are products).
- Because the distribution of the fixed effects is not estimated, we have no basis for estimating these effects in predictions for individuals not in the sample.

Modeling for large data sets

The linear random effects model assumes a simple parametric form for f, which might be too restrictive an assumption; when there is a large number of individuals, a more complex functional form could be supported. Furthermore, K may be very large, requiring model selection, and linear models cannot include variables with missing values as easily as many data mining methods can.

We focus on regression trees. A regression tree is a binary tree, where each non-terminal node is split into two nodes based on the values of a single predictor. This method allows for interactions between variables and can represent a variety of functions of the predictors.

Previous research

Most approaches to extending tree models to longitudinal or clustered data have been based on concepts from multivariate response data (the repeated responses for a particular individual are treated as a multivariate response from that individual, and the splitting criterion is modified accordingly):

- Gillo and Shelly (1974)
- Segal (1992)
- De'Ath (2002) (`mvpart`)
- Larsen and Speckman (2004)
- Loh and Zheng (2013) (`GUIDE`)

Previous research

This approach has several challenges:

- It uses a single set of predictors for all of the observation periods, which means that either time-varying (observation-level) predictors cannot be used, or predictor values from later time periods can potentially be used to predict responses from earlier ones even though that is probably contextually unrealistic.
- It cannot be used for the prediction of future periods for the same individuals in a direct way.
- Missing data is a challenge.

Hajjem et al. (2011) and Sela and Simonoff (2012) independently proposed an approach that accounts for the longitudinal structure of the data while avoiding these difficulties.

"EM"-type algorithm

$$y_{it} = Z_{it}\mathbf{b}_i + f(x_{it1}, ..., x_{itK}) + \varepsilon_{it}$$

If the random effects, $\mathbf{b}_i$, were known, the model implies that we could fit a regression tree to $y_{it} - Z_{it}\mathbf{b}_i$ to estimate f. If the fixed effects, f, were known and can be represented as a linear function, then we could estimate the random effects using a traditional random effects linear model with fixed effects corresponding to the fitted values, $f(x_i)$. This alternation between the estimation of different parameters is reminiscent of (although is not) the EM algorithm, as used by Laird and Ware (1982); for this reason, we call the resulting estimator a Random Effects/EM Tree, or **RE-EM Tree**. Hajjem et al. refer to this as the MERT (mixed effects regression tree) method.

Estimation of a RE-EM Tree

- The fitting of the regression tree uses built-in methods for missing data, such as probabilistic or surrogate split.
- The fitting of the random effects portion of the model can be based on either independence within individuals, or a specified autocorrelation structure.
- Multilevel hierarchies (e.g., classrooms within schools within school districts within counties) are easily handled.
- Nodes are defined at the *observation* level, not the *individual* level; that is, different observations of the same individual end up in different (terminal) nodes. This is why observation-level (time-varying) covariates are easily accommodated.

Transaction data set

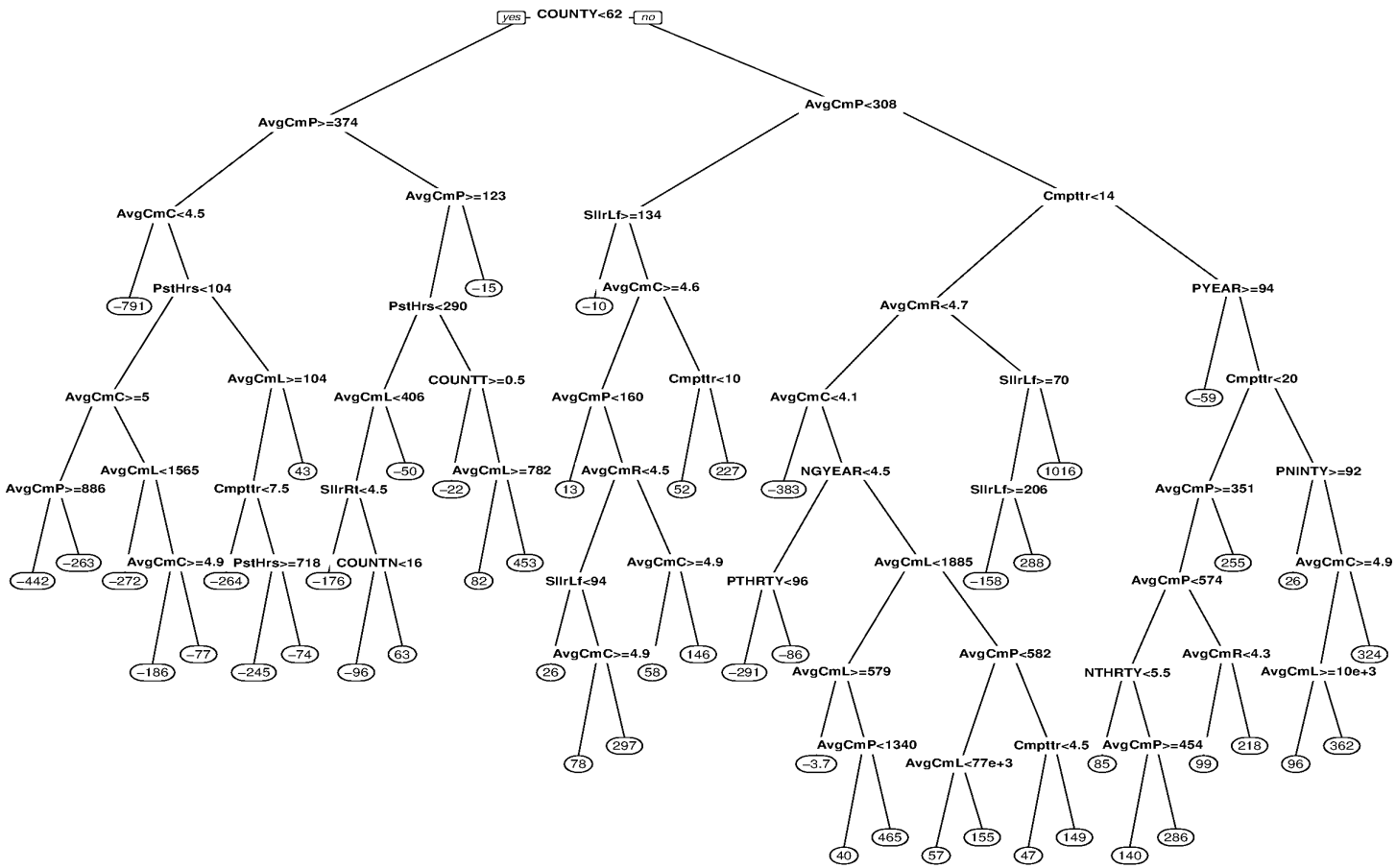
We apply this method to a dataset on third-party sellers on Amazon Web Services to predict the prices at which software titles are sold based on the characteristics of the competing sellers (Ghose, 2005). The goal is to use the tree structure of the RE-EM tree to describe the factors that appear to influence prices. We also use the dataset to compare the predictive performance of the RE-EM tree to that of alternative methods through two types of leave-one-out cross validation.

The data consist of 9484 transactions for 250 distinct software titles; thus, there are $I = 250$ individuals in the panel with a varying number of observations T_i per individual.

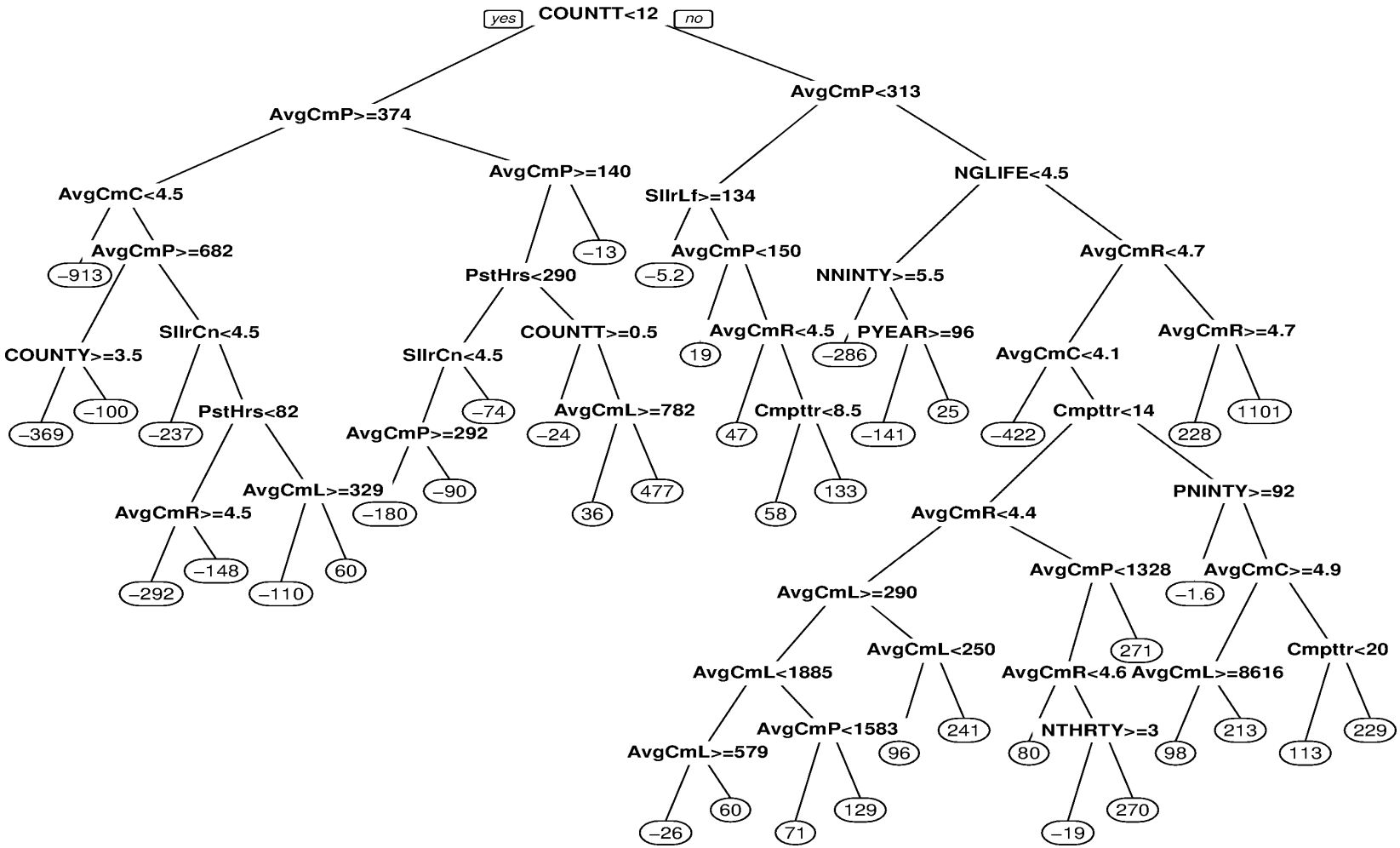
Transaction data set

- Target variable: the price premium that a seller can command (the difference between the price at which the good is sold and the average price of all of the competing goods in the marketplace).
- Predictor variables
  - The seller's own reputation (total number of comments, the number of positive and negative comments received from buyers, the length of time that the seller has been in the marketplace)
  - The characteristics of its competitors (the number of competitors, the quality of competing products, and the average reputation of the competitors, and the average prices of the competing products).

Tree ignoring longitudinal structure



RE-EM Tree


yes
COUNTT<12
no
AvgCmP>=374
AvgCmP<313
AvgCmC<4.5
AvgCmP>=140
SllrLf>=134
NGLIFE<4.5
AvgCmP>=682
−13
AvgCmP<150
AvgCmR<4.7
−913
PstHrs<290
−5.2
NNINTY>=5.5
SllrCn<4.5
COUNTT>=0.5
AvgCmR<4.5
PYEAR>=96
AvgCmR>=4.7
COUNTY>=3.5
SllrCn<4.5
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−286
AvgCmC<4.1
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−74
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Cmpttr<8.5
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−369
−237
PstHrs<82
AvgCmP>=292
−24
47
−141
Cmpttr<14
−422
228
AvgCmL>=329
−90
477
133
PNINTY>=92
AvgCmR>=4.5
−180
36
58
AvgCmR<4.4
−148
60
AvgCmP<1328
AvgCmC>=4.9
−292
−110
AvgCmL>=290
−1.6
AvgCmL<250
271
Cmpttr<20
AvgCmL<1885
AvgCmR<4.6
AvgCmL>=8616
AvgCmP<1583
241
NTHRTY>=3
213
229
AvgCmL>=579
96
80
98
113
60
129
270
−26
71
−19

Cross-validated RMSE accuracy

Method	Excluding Observations	Excluding Titles
Linear Model	95.88	96.92
LM with RE	73.62	461.48
LM with RE - AR(1)	74.75	387.18
`rpart`	69.66	89.38
RE-EM Tree	64.54	88.53
RE-EM Tree - AR(1)	63.88	87.90
FE-EM Tree	65.67	91.10

Results of simulation study

- When the true data generation process is a tree
  - RE-EM tree is best
  - ordinary (`rpart`) tree beats linear models with or without random effects
- When the true data generation process is a linear model
  - linear random effects model is best for small samples
  - RE-EM tree is as good as the linear model with random effects when T or I are large for some types of predictions, and better for others
- When the true data generation is a complex polynomial model with interactions the relative performance of the tree and linear model methods are similar to when it is a linear model.

Results of simulation study

- RE-EM tree provides more accurate estimates of random effects in almost all situations.
- When the true data generation process is a tree RE-EM tree provides best estimates of true fixed effects.
- When the true data generation process is a linear or polynomial model
  - linear random effects model provides best estimates of true fixed effects for small samples
  - RE-EM tree is as good as linear model when T or I are large
- Autocorrelation hurts all models, but hurts linear models more.

Linear mixed effects models and goodness-of-fit

Recall the general mixed effects model

$$y_{it} = Z_{it}\mathbf{b}_i + f(x_{it1}, \ldots, x_{itK}) + \varepsilon_{it}.$$

The most common choice of f is of course the linear model

$$y_{it} = Z_{it}\mathbf{b}_i + X_{it}\boldsymbol{\beta} + \varepsilon_{it},$$

assuming errors ε that are normally distributed with constant variance. This model has the advantage of simplicity of interpretation, but as is always the case, if the assumptions of the model do not hold inferences drawn can be misleading. Such model violations include *nonlinearity* and *heteroscedasticity*. If specific violations are assumed, tests such as likelihood ratio tests can be constructed, but omnibus goodness-of-fit tests would be useful to help identify unspecified model violations.

Regression trees and goodness-of-fit

The idea discussed here is a simple one that has (perhaps) been underutilized through the years: since the errors are supposed to be unstructured if the model assumptions hold, examining the residuals using a method that looks for unspecified structure can be used to identify model violations. A natural method for this is a regression tree.

Miller (1996) proposed using a CART regression tree for this purpose in the context of identifying unmodeled nonlinearity in linear least squares regression, terming it a **diagnostic tree**.

Regression trees and goodness-of-fit

Su, Tsai, and Wang (2009) altered this idea slightly by simultaneously including both linear and tree-based terms in one model, terming it an **augmented tree**, assessing whether the tree-based terms are deemed necessary in the joint model. They also note that building a diagnostic tree using squared residuals as a response can be used to test for heteroscedasticity.

The diagnostic trees are not meant to replace examination of residuals or more focused (and powerful) tests of specific model violations; rather, they are an omnibus tool to add to the data analyst's toolkit to try to help identify unspecified mixed effects model violations.

Proposed method

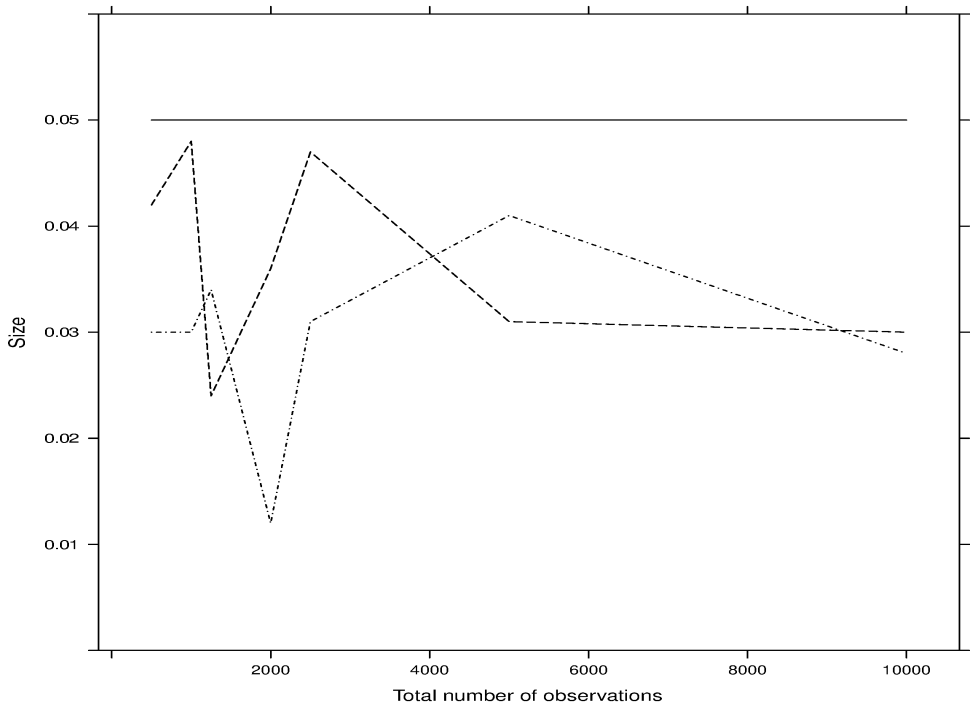
We propose adapting the diagnostic tree idea to longitudinal/clustered data using RE-EM trees as follows:

- Fit the linear mixed effects model.
- Fit a RE-EM tree to the residuals from this model to explore nonlinearity.
- Fit a RE-EM tree to the absolute residuals from the model to explore heteroscedasticity (squared residuals are more non-Gaussian and lead to poorer performance).

A final tree that splits from the root node rejects the null model.

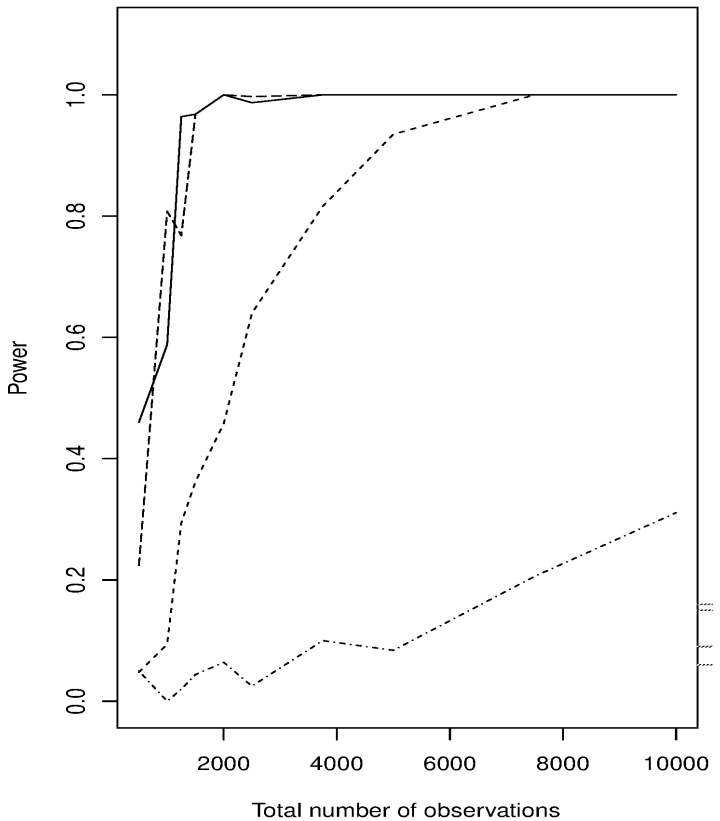
Null size of tests

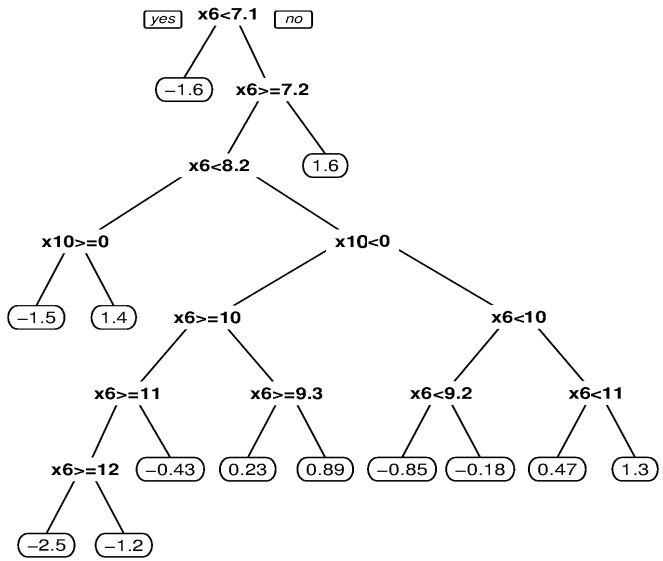
Even though the growing/pruning rules for the tree are not designed to directly control Type I error, it turns out that they do at a roughly .05 level, resulting in a generally conservative test.



Power of nonlinearity test: Different slopes

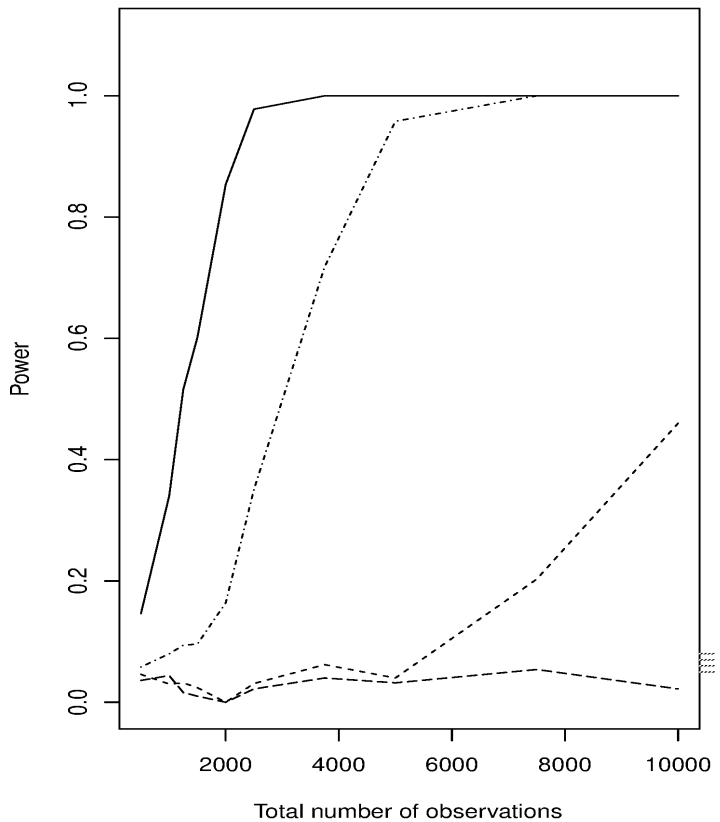
$$E(y) = E_0(y) \pm_{x_{10}} \alpha x_6, \alpha = .25(.25)1$$

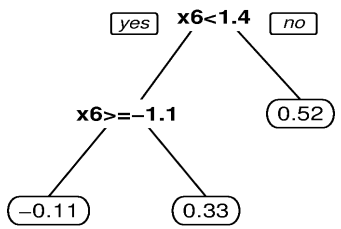




Power of nonlinearity test: Quadratic term

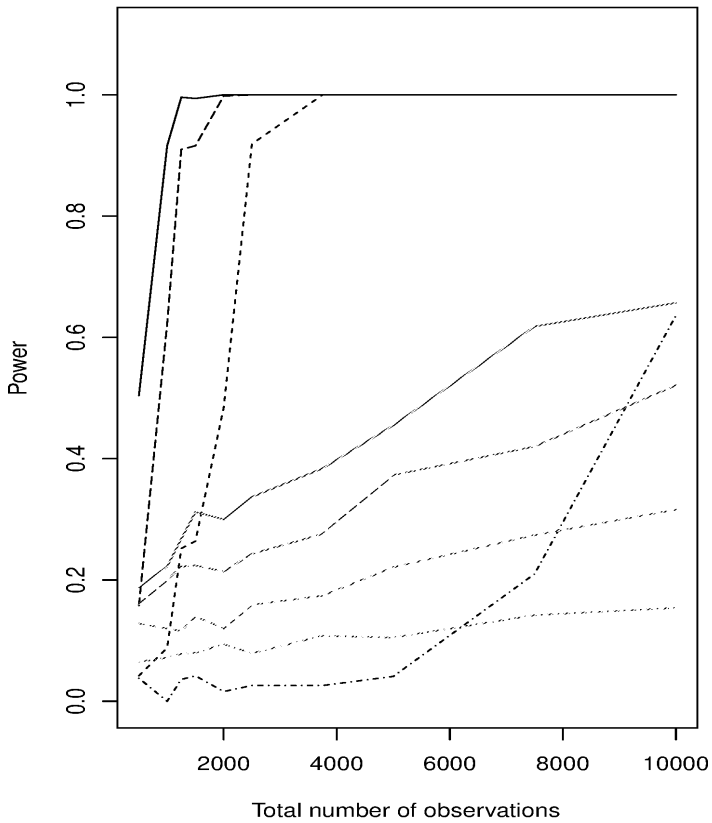
$$E(y) = E_0(y) \pm \alpha x_6^2, \alpha = .05(.05).2, E(x_6) = 0$$

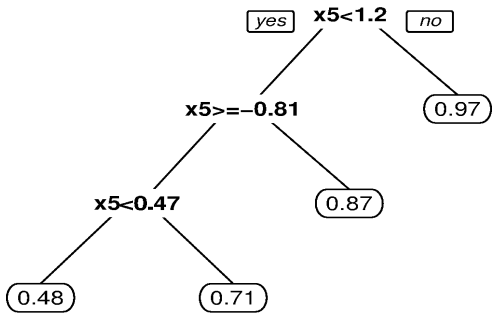




Power of test of heteroscedasticity related to predictor

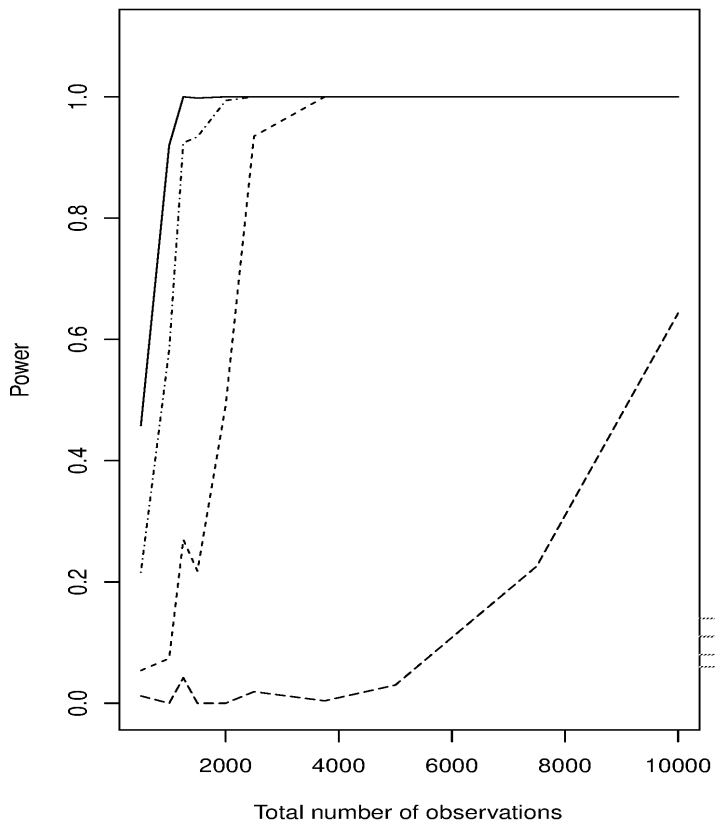
$$\sigma_y^2 = |x_5|^\alpha, \alpha = .125(.125).5\, E(x_5) = 0$$

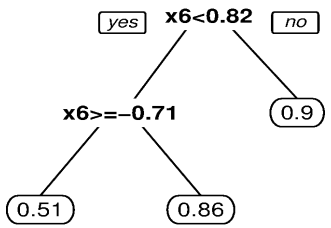




Power of test of heteroscedasticity related to nonpredictor

$$\sigma_y^2 = |x_6|^\alpha, \alpha = .125(.125).5 \; E(x_6) = 0$$



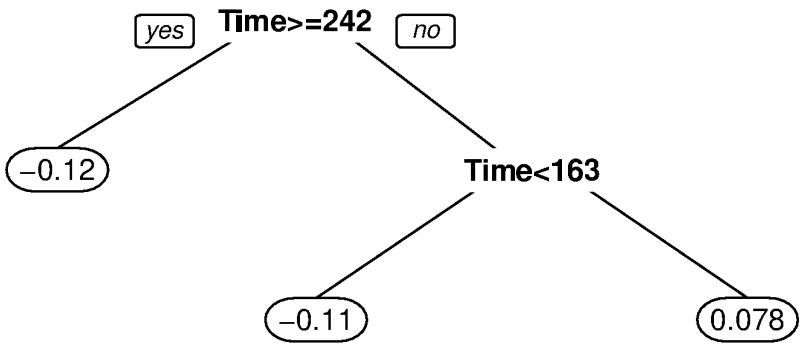


Spruce tree growth

Diggle, Liang, and Zeger (1994) and Venables and Ripley (2002) discuss a longitudinal growth study. The response is the log-size of 79 Sitka spruce trees, two-thirds of which were grown in ozone-enriched chambers, measured at five time points.

First, a linear model based on treatment status and time is fit, but the tree-based nonlinearity test indicates lack of fit related to time.

Test of fit of linear models



A natural alternative model is one allowing for different slopes for the treatment and control groups, but that does not correct the lack of fit.

Treating time as categorical

As the diagnostic trees suggest, the problem is in the linear formulation of the effect of time. If time is treated as a categorical predictor, the apparent lack of fit disappears, as the diagnostic tree has no splits.

An additional interaction of the treatment and (categorical) time effects is statistically significant, but has higher *AIC* and *BIC* values than the additive model, reinforcing that from a practical point of view the fit of the simpler model is adequate.

Heteroscedasticity diagnostic trees for all models do not split.

Variable selection bias

Tree methods like CART suffer from a variable selection (splitting) bias, in that the algorithm is more likely to split on variables with a larger number of possible split points. This bias is introduced because the tree is constructed based on maximization of a splitting criterion over all possible splits simultaneously; that is, the choice of which variable to split on and where the split should be are made in a single step. As a result of this, in general, standard measures of impurity will prefer a variable that has been randomly partitioned into a larger number of values as a candidate for splitting, even though the additional partition is random.

Avoiding variable selection bias

Several authors have proposed approaches that avoid this bias. In the multivariate response / longitudinal framework `GUIDE` (Loh and Zheng, 2013) and `MELT` (Eo and Cho, 2014) use χ^2 goodness-of-fit tests based on residuals to assess whether a variable should be split, with the best split set then found for that variable. In the RE-EM tree formulation, any variable selection bias comes from the use of CART as the underlying tree method using $y_{it} - Z_{it}\hat{\mathbf{b}}_i$ as the responses, but there is no requirement that CART be used for this; if a tree method that has unbiased variable selection is used instead, the resultant RE-EM tree should inherit that lack of bias.

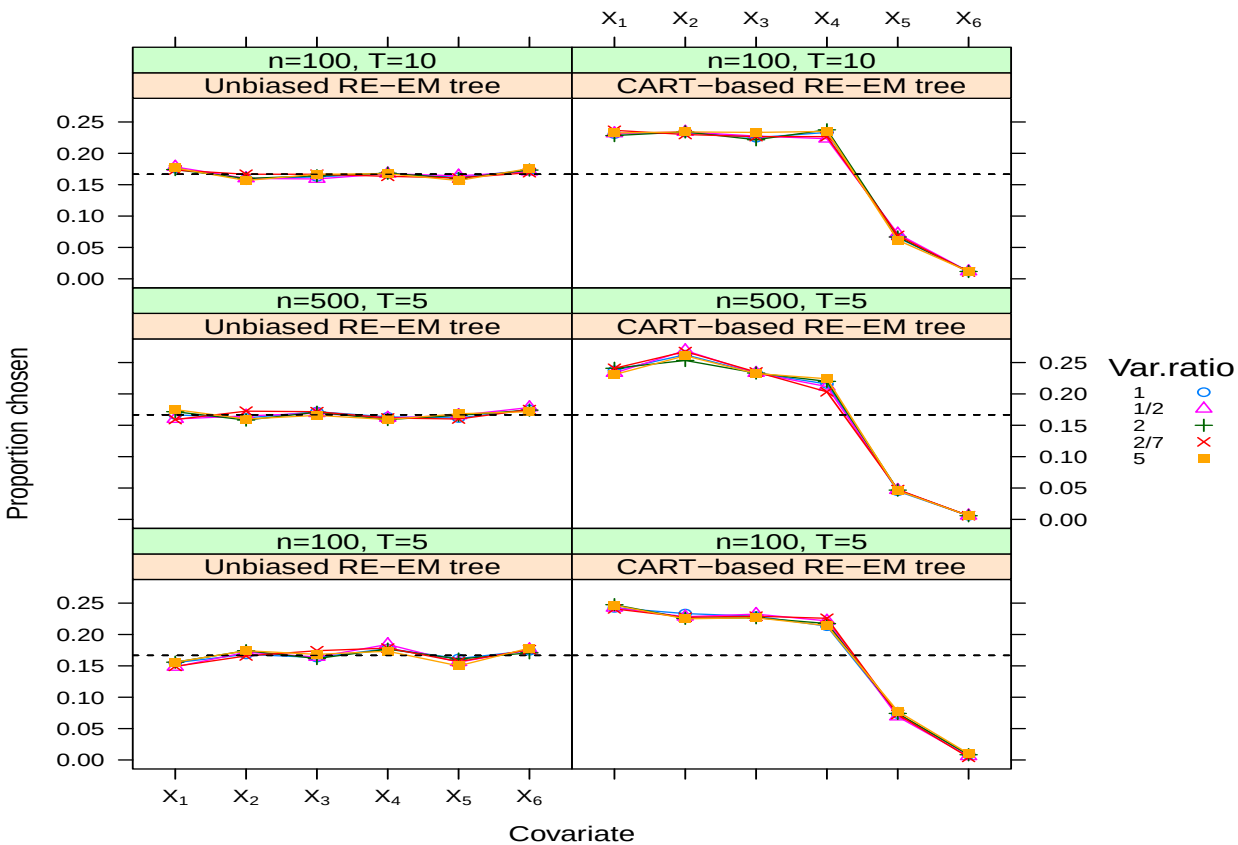
Conditional inference trees

We replace CART with the *conditional inference tree* proposed by Hothorn et al. (2006). This method is based on a hypothesis testing approach, in which the process of choosing variables on which to split is stopped when the hypothesis that all of the conditional distributions of y given X_j equal the unconditional distributions cannot be rejected. The testing is based on a permutation version of each conditional distribution, addressing the bias problem (since the p-value for the test of association of y and X_j is not related to the number of potential splitting points of X_j). The split point itself can be determined by any criterion, and unlike CART, no pruning procedure is necessary (avoiding the randomness of the 10-fold cross-validation pruning procedure).

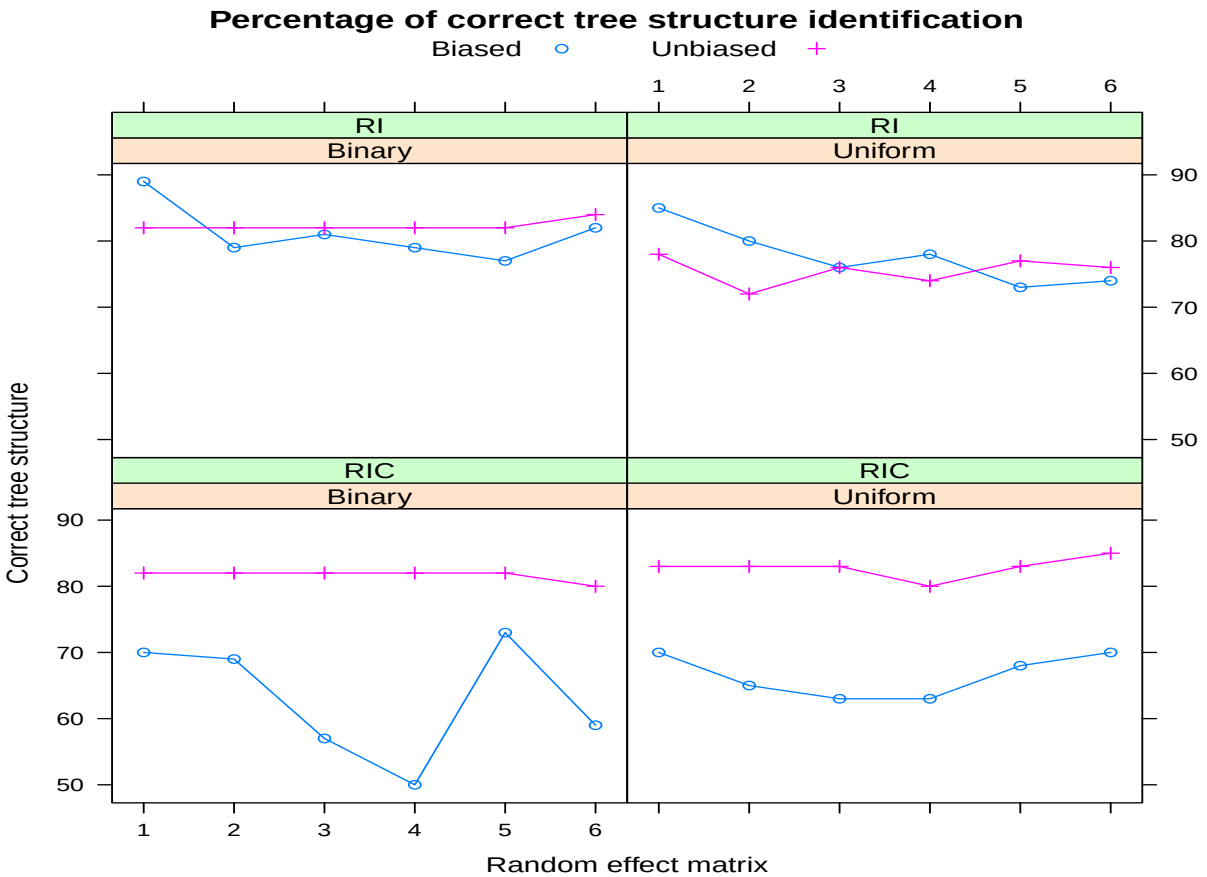
The algorithm that implements this method is available in the R package `party`.

Variable selection properties (bias)

$X_1, \ldots, X_3$ uniform, X_4 missing data, X_5 ordinal, X_6 binary

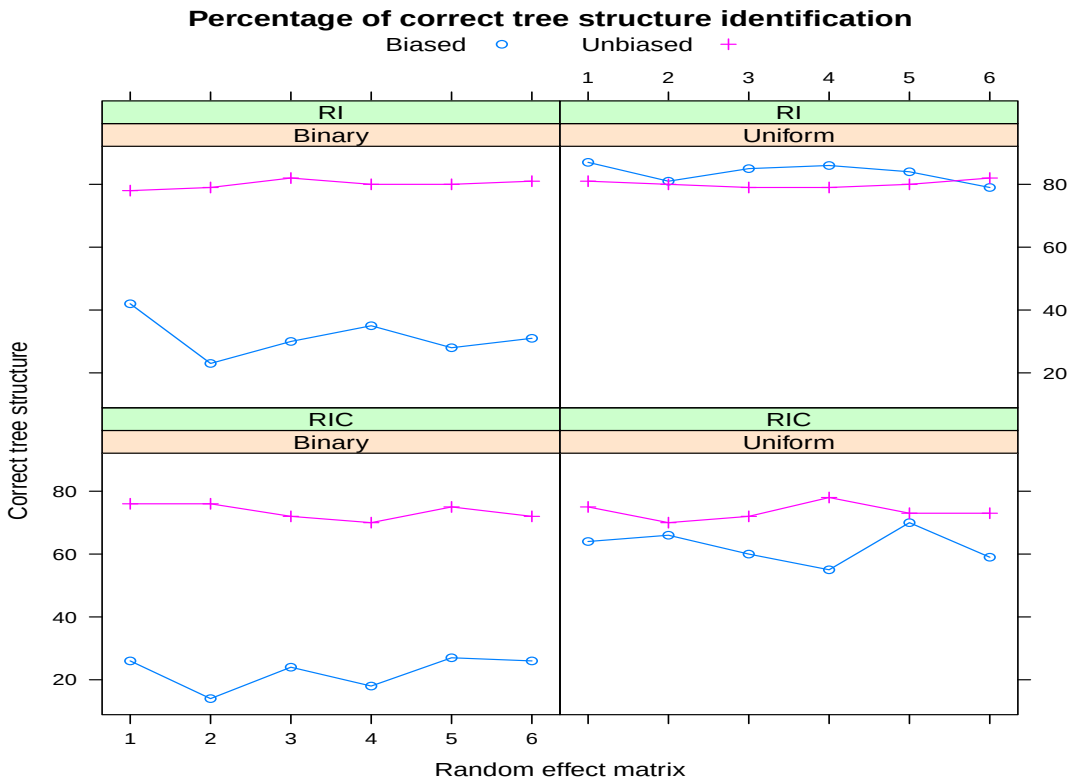


Tree performance with no "competitor"



In all cases the unbiased tree has lower error in estimating fixed effects.

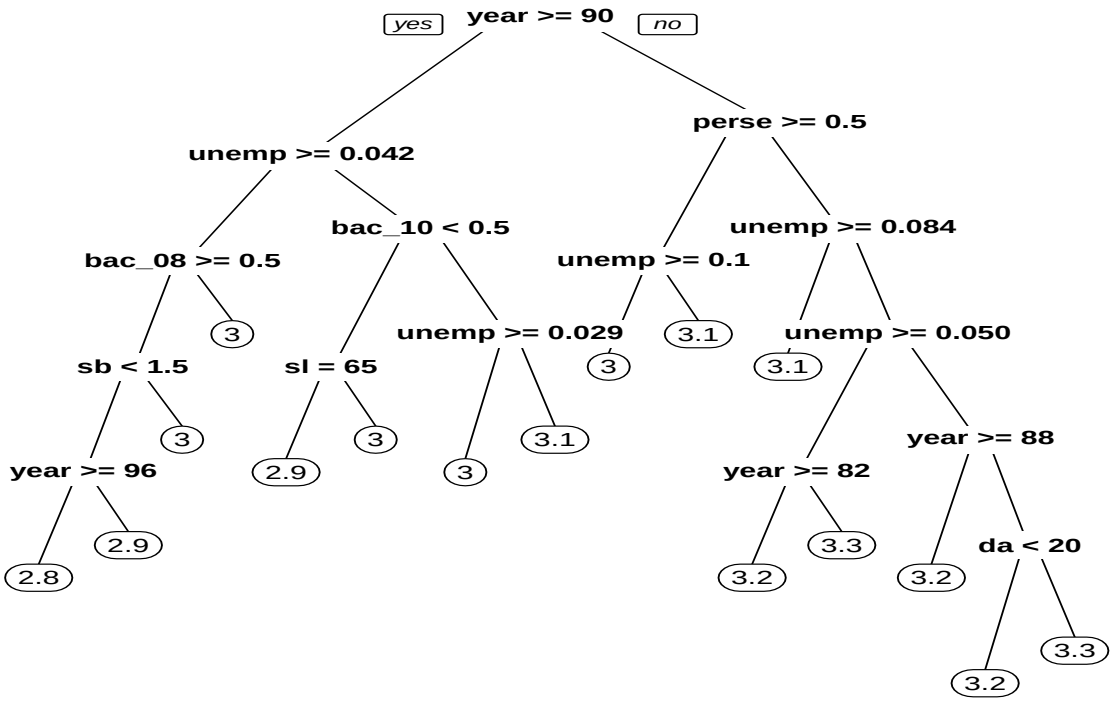
Tree performance with a continuous "competitor"



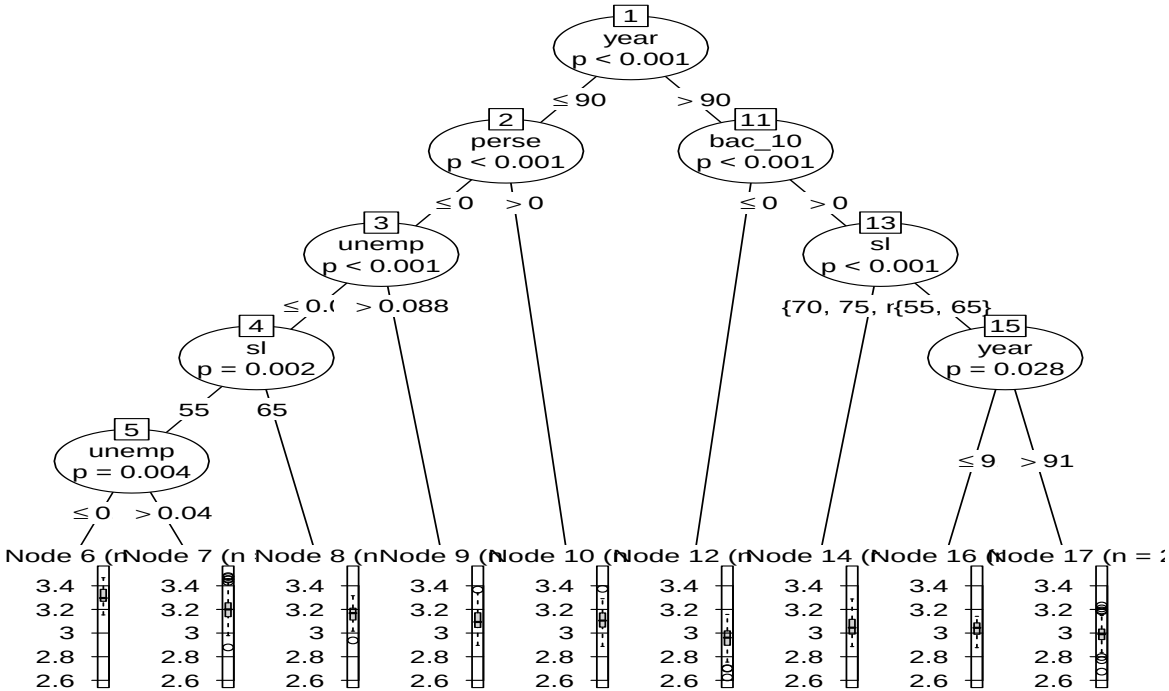
The biased tree fails completely for a random intercept with a binary first split variable.

Logged highway fatality rates

Dee and Sela (2003) discuss state-by-state data examining logged highway fatality rates from 1982-1999 as a function of time, traffic laws, and alcohol-related laws. Here is a CART-based RE-EM tree:



Logged highway fatality rates; unbiased tree



The two trees are broadly similar, having year as the root split variable, and unemployment rate, maximum blood alcohol level allowed, and speed limit in common, but the unbiased tree is a bit simpler.

Cross-validated predictive performance

	Leave-one-observation-out cross-validation		
	Mean	Median	PRMSE
Unbiased RE-EM Tree	0.00954	0.00380	0.09771
CART-based RE-EM Tree	0.01023	0.00389	0.10115
	Leave-one-state-out cross-validation		
	Mean	Median	PRMSE
Unbiased RE-EM Tree	0.28082	0.25225	0.52993
CART-based RE-EM Tree	0.28391	0.25152	0.53283

Future work

- How to extend to ensemble methods such as bagging, boosting, and random forests as a way to improve predictive performance by reducing variability?
- How to generalize this idea to classification trees and non-Gaussian distributions?
- Can tree-based methods be built that jointly model longitudinal and time-to-event data?
- What is the best way to generalize the fitted response from a constant to a functional form, such as a fitted growth curve at each node? [Loh and Zheng, 2013; Eo and Cho, 2014]

Sources

- Sela, R.J. and Simonoff, J.S. (2012), "RE-EM Trees: A Data Mining Approach for Longitudinal and Clustered Data," *Machine Learning*, **86**, 169-207.
- Simonoff, J.S. (2013), "Regression Tree-Based Diagnostics for Linear Multilevel Models," *Statistical Modelling*, **13**, 459-480.
- Fu, W. and Simonoff, J.S. (2014), "Unbiased Regression Trees for Longitudinal Data." Available at SSRN: `http://ssrn.com/abstract=2399976`.

The `R` package `REEMtree` used to construct RE-EM trees based on `rpart` is available from CRAN.