Model-Based Recursive Partitioning for Detecting Interaction Effects in Subgroups

Achim Zeileis, Torsten Hothorn, Kurt Hornik

http://eeecon.uibk.ac.at/~zeileis/

Overview

- Motivation: Trees, leaves, and branches
- Model-based recursive partitioning
  - Model estimation
  - Tests for parameter instability
  - Segmentation
  - Pruning
- Application: Treatment effect for chronic disease
- Summary

Motivation: Trees

Breiman (2001, *Statistical Science*) distinguishes two cultures of statistical modeling.

- **Data models:** Stochastic models, typically parametric.
- **Algorithmic models:** Flexible models, data-generating process unknown.

Example: Recursive partitioning models dependent variable Y by "learning" a partition w.r.t explanatory variables $Z_1, \dots, Z_l$.

Key features:

- Predictive power in nonlinear regression relationships with "automatic interaction detection".
- Interpretability (enhanced by visualization), i.e., no "black box" methods.

Motivation: Leaves

Typically: Simple models for univariate Y, e.g., mean or proportion.

Examples: CART and C4.5 in statistical and machine learning, respectively.

Problems: For classical tree algorithms.

- No concept of “significance”, possibly biased variable selection.
- No complex (parametric) models in leaves.
- Many different tree algorithms for different types of data.

Here: Synthesis of parametric data models and algorithmic tree models.

- Fitting local models by partitioning of the sample space.
- Based on statistical hypothesis tests for parameter instability.

Motivation: Branches

Base algorithm: Growth of branches from the roots to the leaves of the tree follows a generic *recursive partitioning* algorithm.

1. Fit a (possibly very simple) model for the response Y.
2. Assess association of Y and each Z_j.
3. Split sample along the Z_{j^*} with strongest association: Choose breakpoint with highest improvement of the model fit.
4. Repeat steps 1–3 recursively in the subsamples until some stopping criterion is met.

Here: Segmentation (3) of parametric models (1) with additive objective function using parameter instability tests (2) and associated statistical significance (4).

Model-based recursive partitioning: Estimation

Models: $\mathcal{M}(Y, \theta)$ with (potentially) multivariate observations $Y \in \mathcal{Y}$ and k-dimensional parameter vector $\theta \in \Theta$.

Parameter estimation: $\widehat{\theta}$ by optimization of objective function $\Psi(Y, \theta)$ for n observations Y_i ($i = 1, \dots, n$):

$$\widehat{\theta} \quad = \quad \underset{\theta \in \Theta}{\operatorname{argmin}} \sum_{i=1}^{n} \Psi(Y_i, \theta).$$

Special cases: Maximum likelihood (ML), weighted and ordinary least squares (OLS and WLS), quasi-ML, and other M-estimators.

Central limit theorem: If there is a true parameter θ_0 and given certain weak regularity conditions, $\hat{\theta}$ is asymptotically normal with mean θ_0 and sandwich-type covariance.

Model-based recursive partitioning: Estimation

Estimating function: $\widehat{\theta}$ can also be defined in terms of

$$\sum_{i=1}^{n} \psi(Y_i, \widehat{\theta}) = 0,$$

where $\psi(Y, \theta) = \partial \Psi(Y, \theta)/\partial \theta$.

Idea: In many situations, a single global model $\mathcal{M}(Y, \theta)$ that fits **all** n observations cannot be found. But it might be possible to find a partition w.r.t. the variables $Z = (Z_1, \dots, Z_l)$ so that a well-fitting model can be found locally in each cell of the partition.

Tool: Assess parameter instability w.r.t to partitioning variables $Z_j \in \mathcal{Z}_j$ ($j = 1, \dots, l$).

Model-based recursive partitioning: Tests

Generalized M-fluctuation tests capture instabilities in $\widehat{\theta}$ for an ordering w.r.t Z_j.

Basis: Empirical fluctuation process of cumulative deviations w.r.t. to an ordering $\sigma(Z_{ij})$.

$$W_j(t, \widehat{\theta}) \quad = \quad \widehat{V}^{-1/2} n^{-1/2} \sum_{i=1}^{\lfloor nt \rfloor} \psi(Y_{\sigma(Z_{ij})}, \widehat{\theta}) \qquad (0 \leq t \leq 1)$$

Functional central limit theorem: Under parameter stability $W_j(\cdot, \widehat{\theta}) \xrightarrow{d} W^0(\cdot)$, where W^0 is a k-dimensional Brownian bridge.

Model-based recursive partitioning: Tests

Test statistics: Scalar functional $\lambda(W_j)$ that captures deviations from zero.

Null distribution: Asymptotic distribution of $\lambda(W^0)$.

Special cases: Class of test encompasses many well-known tests for different classes of models. Certain functionals λ are particularly intuitive for numeric and categorical Z_j, respectively.

Advantage: Model $\mathcal{M}(Y, \widehat{\theta})$ just has to be estimated once. Empirical estimating functions $\psi(Y_i, \widehat{\theta})$ just have to be re-ordered and aggregated for each Z_j.

Model-based recursive partitioning: Tests

Splitting numeric variables: Assess instability using sup*LM* statistics.

$$\lambda_{\sup LM}(W_j) \quad = \quad \max_{i=\underline{i},\dots,\bar{\imath}} \left(\frac{i}{n} \cdot \frac{n-i}{n} \right)^{-1} \left\| W_j \left(\frac{i}{n} \right) \right\|_2^2 .$$

Interpretation: Maximization of single shift *LM* statistics for all conceivable breakpoints in $[\underline{i}, \bar{\imath}]$.

Limiting distribution: Supremum of a squared, *k*-dimensional tied-down Bessel process.

Model-based recursive partitioning: Tests

Splitting categorical variables: Assess instability using χ^2 statistics.

$$\lambda_{\chi^2}(W_j) \quad = \quad \sum_{c=1}^{C} \frac{n}{|I_c|} \left\| \Delta_{I_c} W_j \left(\frac{i}{n} \right) \right\|_2^2$$

Feature: Invariant for re-ordering of the C categories and the observations within each category.

Interpretation: Captures instability for split-up into C categories.

Limiting distribution: χ^2 with $k \cdot (C - 1)$ degrees of freedom.

Model-based recursive partitioning: Segmentation

Goal: Split model into $b = 1, \dots, B$ segments along the partitioning variable Z_j associated with the highest parameter instability. Local optimization of

$$\sum_{b} \sum_{i \in I_b} \Psi(Y_i, \theta_b).$$

$B = 2$: Exhaustive search of order $O(n)$.

$B > 2$: Exhaustive search is of order $O(n^{B-1})$, but can be replaced by dynamic programming of order $O(n^2)$. Different methods (e.g., information criteria) can choose B adaptively.

Here: Binary partitioning.

Model-based recursive partitioning: Pruning

Pruning: Avoid overfitting.

Pre-pruning: Internal stopping criterion. Stop splitting when there is no significant parameter instability.

Post-pruning: Grow large tree and prune splits that do not improve the model fit (e.g., via cross-validation or information criteria).

Here: Pre-pruning based on Bonferroni-corrected p values of the fluctuation tests.

Application: Treatment effect for chronic disease

Task: Identify groups of chronic disease patients with different treatment effects.

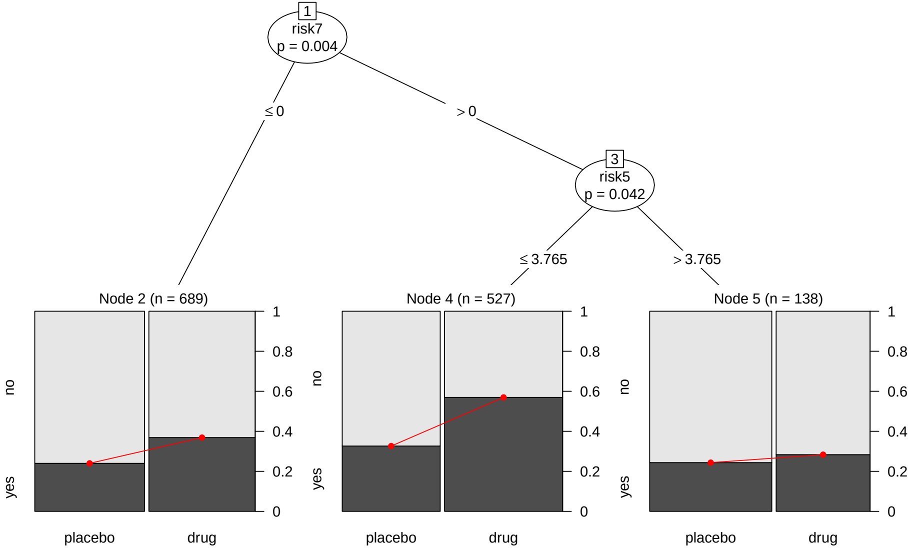
Source: Anonymized data from consulting project.

Model: Logistic regression estimated by maximum likelihood.

- Response: Improvement (yes/no) of chronic disease for 1354 patients after treatment over several weeks.
- Regressor: Treatment (active drug/placebo).
- Partitioning variables: 11 variables that describe disease status of patients. Lower values indicate more severe forms of the disease.

Result: Treatment most effective for certain intermediate forms.

Application: Treatment effect for chronic disease



Application: Treatment effect for chronic disease

Model-based recursive partitioning:

- Coefficient estimates for regressors.
- Parameter instability tests for partitioning variables (bold = significant at adjusted 5% level, underlined = smallest *p* value).

	Regressors		Partitioning variables					
	(const.)	treatment	risk4	risk5	risk7	risk9	risk10	...
1	−0.99	0.77	13.05	16.01	**<u>22.02</u>**	1.48	13.03	
2	−1.15	0.62	<u>12.57</u>	9.64	3.85	0.06	8.94	
3	−0.82	0.90	6.96	**<u>17.01</u>**	2.53	2.14	13.84	...
4	−0.72	1.00	2.84	6.46	2.51	0.50	<u>12.78</u>	
5	−1.13	0.21	3.96	0.98	3.54	<u>6.10</u>	3.14	

Summary

- Synthesis of parametric data models and algorithmic tree models.
- Based on modern class of parameter instability tests.
- Aims to minimize clearly defined objective function by greedy forward search.
- Can be applied to general class of parametric models: generalized linear models, psychometric models (e.g., Rasch, Bradley-Terry), models for location and scale, etc.
- Automatic interaction detection of effects in subgroups.
- Alternative to traditional means of model specification, especially for variables with unknown association.
- Object-oriented implementation freely available: Extension for new models requires some coding, though.

References

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

Zeileis A, Hornik K (2007). "Generalized M-Fluctuation Tests for Parameter Instability." *Statistica Neerlandica*, **61**(4), 488–508. `doi:10.1111/j.1467-9574.2007.00371.x`

Hothorn T, Hornik K, Strobl C, Zeileis A (2013). ***party**: A Laboratory for Recursive Partytioning*. R package version 1.0-7. `http://CRAN.R-project.org/package=party`