

# **Model-Based Recursive Partitioning**

Achim Zeileis

http://statmath.wu-wien.ac.at/~zeileis/

### **Overview**

- Motivation: Trees and leaves
- Methodology
  - Model estimation
  - Tests for parameter instability
  - Segmentation
  - Pruning
- Applications
  - Costly journals
  - Beautiful professors
  - Choosey students
- Software

### **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  $Z_1, \ldots, Z_l$ .

### Key features:

- Predictive power in nonlinear regression relationships.
- 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.

**Idea:** More complex models for multivariate Y, e.g., multivariate normal model, regression models, etc.

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

**Goal:** Fitting local models by partitioning of the sample space.

## **Recursive partitioning**

### Base algorithm:

- Fit model for 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.
- Repeat steps 1–3 recursively in the sub-samples 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).

### 1. Model 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, ..., n):

$$\widehat{\theta}$$
 = 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  $\theta_0$  and given certain weak regularity conditions,  $\hat{\theta}$  is asymptotically normal with mean  $\theta_0$  and sandwich-type covariance.

### 1. Model 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  $Z=(Z_1,\ldots,Z_l)$  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  $Z_j \in \mathcal{Z}_j \ (j = 1, ..., I)$ .

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  $\sigma(Z_{ij})$ .

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

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

**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  $\lambda$  are particularly intuitive for numeric and categorical  $Z_i$ , 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  $Z_j$ .

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

$$\lambda_{\text{SUPLM}}(W_j) = \max_{i=\underline{i},\dots,\overline{i}} \left(\frac{i}{n} \cdot \frac{n-i}{n}\right)^{-1} \left|\left|W_j\left(\frac{i}{n}\right)\right|\right|_2^2.$$

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

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

**Splitting categorical variables:** Assess instability using  $\chi^2$  statistics.

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

**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:**  $\chi^2$  with  $k \cdot (C-1)$  degrees of freedom.

## 3. Segmentation

**Goal:** Split model into b = 1, ..., 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.

### 4. 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.

## **Costly journals**

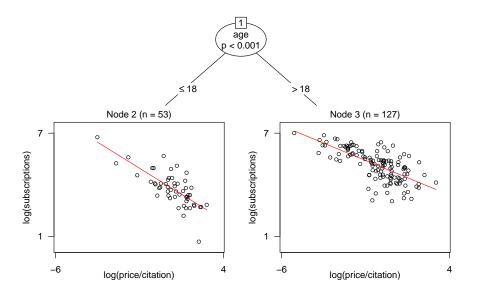
**Task:** Price elasticity of demand for economics journals.

**Source:** Bergstrom (2001, *Journal of Economic Perspectives*) "Free Labor for Costly Journals?", used in Stock & Watson (2007), *Introduction to Econometrics*.

Model: Linear regression via OLS.

- Demand: Number of US library subscriptions.
- Price: Average price per citation.
- Log-log-specification: Demand explained by price.
- Further variables without obvious relationship: Age (in years), number of characters per page, society (factor).

## **Costly journals**



## **Costly journals**

### **Recursive partitioning:**

	Regressors		Partitioning variables				
	(Const.)	log(Pr./Cit.)	Price	Cit.	Age	Chars	Society
1	4.766	-0.533	3.280	5.261	42.198	7.436	6.562
	< 0.001	< 0.001	0.660	0.988	< 0.001	0.830	0.922
2	4.353	-0.605	0.650	3.726	5.613	1.751	3.342
	< 0.001	< 0.001	0.998	0.998	0.935	1.000	1.000
3	5.011	-0.403	0.608	6.839	5.987	2.782	3.370
	< 0.001	< 0.001	0.999	0.894	0.960	1.000	1.000

(Wald tests for regressors, parameter instability tests for partitioning variables.)

**Task:** Correlation of beauty and teaching evaluations for professors.

**Source:** Hamermesh & Parker (2005, *Economics of Education Review*). "Beauty in the Classroom: Instructors' Pulchritude and Putative Pedagogical Productivity."

Model: Linear regression via WLS.

- Response: Average teaching evaluation per course (on scale 1–5).
- Explanatory variables: Standardized measure of beauty and factors gender, minority, tenure, etc.
- Weights: Number of students per course.

	All	Men	Women
(Constant)	4.216	4.101	4.027
Beauty	0.283	0.383	0.133
Gender (= w)	-0.213		
Minority	-0.327	-0.014	-0.279
Native speaker	-0.217	-0.388	-0.288
Tenure track	-0.132	-0.053	-0.064
Lower division	-0.050	0.004	-0.244
$R^2$	0.271	0.316	

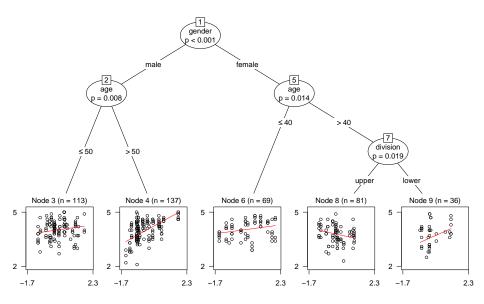
(Remark: Only courses with more than a single credit point.)

#### Hamermesh & Parker:

- Model with all factors (main effects).
- Improvement for separate models by gender.
- No association with age (linear or quadratic).

#### Here:

- Model for evaluation explained by beauty.
- Other variables as partitioning variables.
- Adaptive incorporation of correlations and interactions.



### Recursive partitioning:

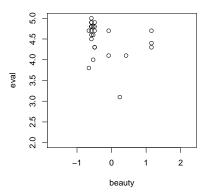
	(Const.)	Beauty
3	3.997	0.129
4	4.086	0.503
6	4.014	0.122
8	3.775	-0.198
9	3.590	0.403

### Model comparison:

<b>-</b>			
Model	$R^2$	Parameters	
full sample	0.271	7	
nested by gender	0.316	12	
recursively partitioned	0.382	10 + 4	

### Single credit courses:

- Different type of courses: Yoga, aerobic, etc.
- Associated with second strongest instability (after gender).
- Sub-samples too small for separated models: 18 (m), 9 (f).



## **Choosy students**

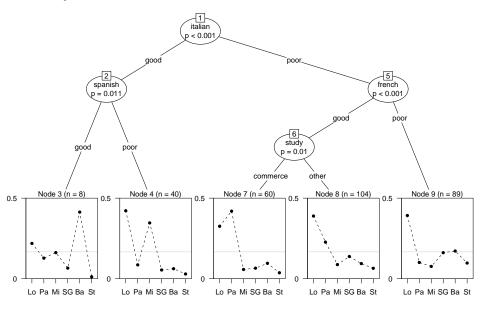
**Task:** Choice of university in student exchange programmes.

**Source:** Dittrich, Hatzinger, Katzenbeisser (1998, *Journal of the Royal Statistical Society C*). "Modelling the Effect of Subject-Specific Covariates in Paired Comparison Studies with an Application to University Rankings."

**Model:** Paired comparison via Bradley-Terry(-Luce).

- Ranking of six european management schools: London (LSE),
   Paris (HEC), Milano (Luigi Bocconi), St. Gallen (HSG), Barcelona (ESADE), Stockholm (HHS).
- Interviews with about 300 students from WU Wien.
- Additional information: Gender, studies, foreign language skills.

## **Choosy students**



# **Choosy students**

### Recursive partitioning:

	London	Paris	Milano	St. Gallen	Barcelona	Stockholm
3	0.22	0.13	0.16	0.07	0.41	0.01
4	0.42	0.09	0.35	0.05	0.06	0.03
7	0.33	0.42	0.06	0.07	0.10	0.04
8	0.39	0.23	0.09	0.14	0.09	0.06
9	0.39	0.10	0.08	0.16	0.17	0.10

(Standardized ranking from Bradley-Terry model.)

### **Software**

**Implementation:** In R system for statistical computing.

- Object-oriented implementation of model-based recursive partitioning in function mob() from package party.
- Underlying inference methods in package strucchange.
- Convenient interfaces for linear regression (lm.fit()), generalized linear models (glm.fit()), and survival regression (survreg()) are readily available.
- Currently: Hand-crafted code for Bradley-Terry model (interfacing glm.fit()), not in package.

### **Software**

#### Extension requirements:

- S4 "StatModel" objects (modeltools package): Separate data handling (in particular, formula processing) from model fitting.
- Fitted models must provide methods: estfun(), weights(), reweight() (at least for 0/1 weights), and extractor for objective function (default: deviance()).
- Further methods are re-used (if available): print(), predict(), coef(), summary(), residuals(), logLik().

### Easy if: Model already available in R with

- Fitted model class with all the usual extractor functions.
- Access to empirical estimating functions (estfun() method).
- In addition to formula interface (à la lm()): Fitting function (à la lm.fit()) that returns sufficiently post-processed output.

### **Software**

#### Caveats:

- For visualization: Panel-generating function for **grid** graphics.
- mob() interprets weights as case weights (and expects the "StatModel" objects to do the same).
- Non-standard formula processing for multivariate responses.
- Hopefully: New model/formula interface soon on R-Forge.

**Example:** Simple implementation of basic Bradley-Terry model.

- Interfaces: btl() and btl.fit() plus methods.
- Workhorse: Set up design matrix, call glm.fit() with family = binomial(), suitably aggregate results.
- Glue code: S4 "BTL" object with few additional methods.

#### **Artificial data:**

```
R> pc <- rbind(
+ c(1, 1, 1), # a > b > c
+ c(1, 1, 0), # a > c > b
+ c(1, 0, 0), # c > a > b
+ c(1, 1, 1) # a > b > c
+ )
R> colnames(pc) <- c("ab", "ac", "bc")
```

Question: Proper data structures for paired comparison data?

**Ideally:** pc should be treated like a *vector* of length 4 (# subjects) with suitable meta-data that reflects # objects, labels, printing, etc.

**Interfaces**: Formula interface and workhorse fitting function.

```
R> btl(pc ~ 1)
Bradley-Terry-Luce model
Coefficients:
 1.7542 - 0.4158
Standardized latent ranking:
     a b
0.7769 0.0887 0.1344
R> pc_btl <- btl.fit(pc)
R> class(pc_btl)
[1] "btl"
```

```
R> coef(pc_btl)
 1.7541765 -0.4158042
R> coef(pc_btl, log = FALSE)
0.77686224 0.08870199 0.13443577
R> estfun(pc_btl)
[1.] 0.2500030 0.4999987
[2,] 0.2500030 -0.5000014
[3,] -0.7500083 -0.5000014
[4.] 0.2500030 0.4999987
R> deviance(pc_btl)
[1] 11.36700
R> logLik(pc_btl)
'log Lik.' -5.683498 (df=2)
```

```
R> btl.fit(y = pc, weights = c(1, 1, 1, 0))
Bradley-Terry-Luce model

Coefficients:
    a    b
1.145 -1.145

Standardized latent ranking:
    a    b    c
0.70450 0.07133 0.22417
```

```
Interface: "StatModel" glue code.
R> class(BTL)
[1] "StatModel"
attr(,"package")
[1] "modeltools"
R> mf <- ModelEnvFormula(ab + ac + bc ~ 1,
+ data = as.data.frame(pc))
R> pc_BTL <- fit(BTL, mf)
R> class(pc_BTL)
[1] "BTL" "btl"
R> pc_BTL
BTL coefficients:
 1.7542 - 0.4158
```

```
R > pc_BTL2 < - reweight(pc_BTL, weights = c(1, 1, 1, 0))
R> weights(pc_BTL2)
[1] 1 1 1 0
R> coef(pc_BTL2)
 1.145071 -1.145071
R> estfun(pc_BTL2)
              a
[1,] 0.3333340 0.6666672
[2,] 0.3333340 -0.3333340
[3,] -0.6666672 -0.3333340
[4,] 0.0000000 0.0000000
```

```
R> load("cems.rda")
R> cems <- cems[!apply(sapply(cems[,1:15], is.na), 1, all),]
R > cems mob < -mob(ab + ac + ad + ae + af + bc + bd + be +
     bf + cd + ce + cf + de + df + ef ~ 1 | study + english +
     french + spanish + italian + work + gender + intdegree,
+
     data = cems, model = BTL, na.action = na.pass,
     control = mob_control(minsplit = 5))
+
R> plot(cems_mob, terminal_panel = node_btlplot,
     tnex = 2, tp_args = list(yscale = c(0, 0.5),
+
     names = c("Lo", "Pa", "Mi", "SG", "Ba", "St")))
R> coef(cems mob)
3 2.915557 2.37530103
                       2.6132469 1.7116796 3.5496433
4 2.657933 1.06913836
                       2.4611060 0.6068164 0.7413380
7 2.174962 2.42810393 0.4400174 0.5704167 0.9507593
8 1.794987 1.25646206 0.3024828 0.7576933 0.3729114
9 1.394938 0.03678015 -0.2427147 0.5071161 0.5702408
```

### **Summary**

#### Model-based recursive partitioning:

- Synthesis of classical 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 general class of parametric models.
- 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 but is limited if interfaced model is well designed.