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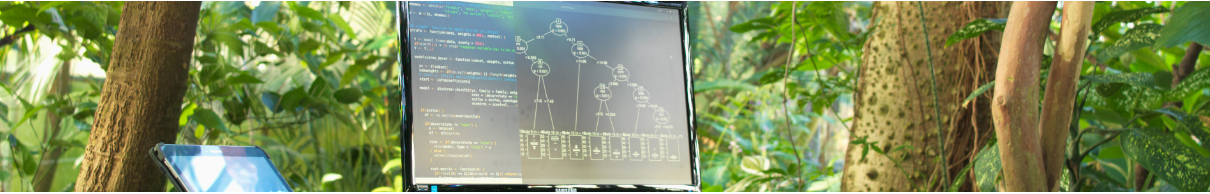

Parties, Models, Mobsters

Methods and Software for Model-Based Recursive Partitioning

Achim Zeileis

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

Motivation

Motivation: Trees

Breiman (2001): Distinguishes two cultures of statistical modeling (*Statistical Science, 16(3), 199–215*).

- **Data models:** Stochastic models, typically parametric.
  $\rightarrow$ Classical strategy in statistics. Regression models are still the workhorse for many empirical analyses.
- **Algorithmic models:** Flexible models, data-generating process unknown.
  $\rightarrow$ Less applications in many fields, e.g., social sciences or economics.

Classical example: Trees, i.e., modeling of dependent variable y by "learning" a recursive partition w.r.t explanatory variables $z_1, \dots, z_l$.

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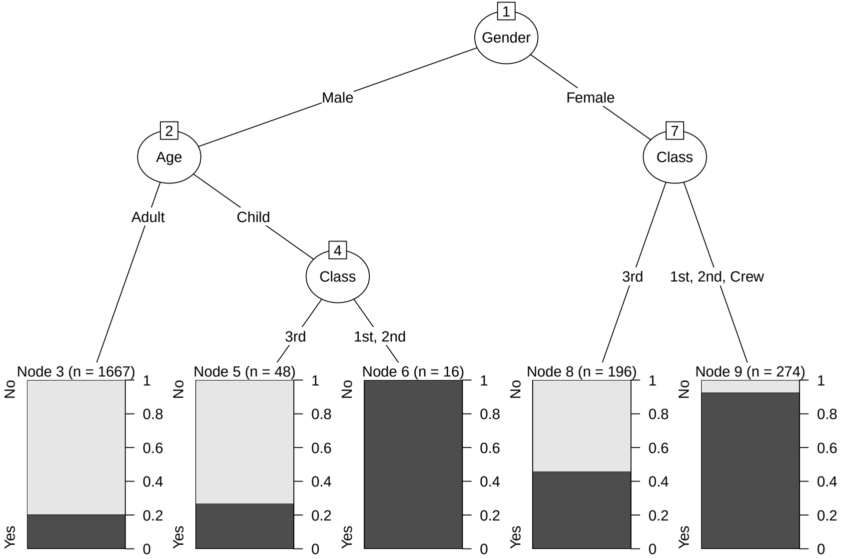
Classical example: Trees, i.e., modeling of dependent variable y by "learning" a recursive partition w.r.t explanatory variables $z_1, \ldots, z_l$.

Example: Recursive partitioning (RPart) for dependence of survival on the Titanic w.r.t. gender, age, and class of passengers.

Motivation: Trees



Motivation: Leaves

Key features:

1. Predictive power in nonlinear regression relationships.
2. Interpretability (enhanced by visualization), i.e., no “black box” methods.

Typically: Simple models for univariate y, e.g., mean.

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Key features:

1. Predictive power in nonlinear regression relationships.
2. Interpretability (enhanced by visualization), i.e., no “black box” methods.

Typically: Simple models for univariate y, e.g., mean.

Idea: More complex models for more complex y, e.g., regression models, multivariate normal model, item responses, etc.

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

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

Model-based recursive partitioning

Model-based recursive partitioning

MOB algorithm:

1. Fit the parametric model in the current subsample.
2. Assess the stability of the parameters across each splitting variable z_j.
3. Split sample along the z_{j^*} with strongest instability: Choose breakpoint with highest improvement of the model fit.
4. Repeat steps 1–3 recursively in the subsamples until some stopping criterion is met.

Model-based recursive partitioning

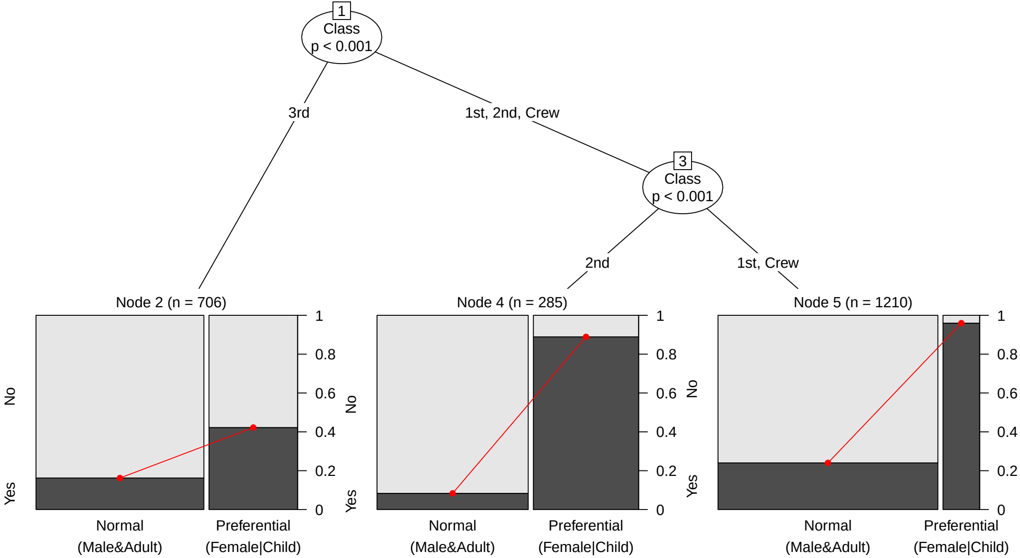
Example: Logistic regression, assessing differences in the effect of "preferential treatment" ("women and children first"?) in the Titanic survival data.

In R: Generalized linear model tree with binomial family (and default logit link).

```
R> library("partykit")
R> mb <- glmtree(Survived ~ Treatment | Age + Gender + Class,
+    data = ttnc, family = binomial, alpha = 0.05, prune = "BIC")
R> plot(mb)
R> print(mb)
```

Result: Log-odds ratio of survival given treatment differs across classes (slope), as does the survival probability of male adults (intercept).

Model-based recursive partitioning



Model-based recursive partitioning

```
Generalized linear model tree (family: binomial)

Model formula:
Survived ~ Treatment | Age + Gender + Class

Fitted party:
[1] root
|   [2] Class in 3rd: n = 706
|                (Intercept) TreatmentPreferential
|                     -1.641                 1.327
|   [3] Class in 1st, 2nd, Crew
|   |   [4] Class in 2nd: n = 285
|   |                (Intercept) TreatmentPreferential
|   |                     -2.398                 4.477
|   |   [5] Class in 1st, Crew: n = 1210
|   |                (Intercept) TreatmentPreferential
|   |                     -1.152                 4.318

Number of inner nodes:    2
Number of terminal nodes: 3
Number of parameters per node: 2
Objective function (negative log-likelihood): 1061
```

1. Model estimation

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

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

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

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

1. Model estimation

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

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

where $\psi(y, x, \theta) = \partial \Psi(y, x, \theta)/\partial\theta$ is the model score function.

Central limit theorem: If there is a true parameter θ_0 and given certain weak regularity conditions

$$\sqrt{n}(\widehat{\theta} - \theta_0) \quad \xrightarrow{\mathrm{d}} \quad \mathcal{N}(0, V(\theta_0)),$$

where $V(\theta_0) = \{A(\theta_0)\}^{-1} B(\theta_0) \{A(\theta_0)\}^{-1}$. A and B are the expectation of the derivative of ψ and the variance of ψ, respectively.

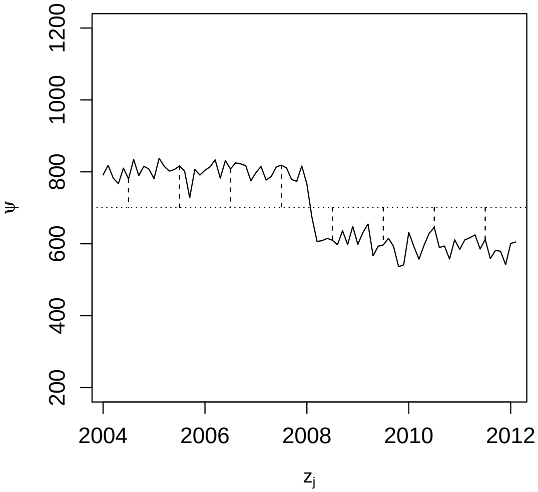
1. Model estimation

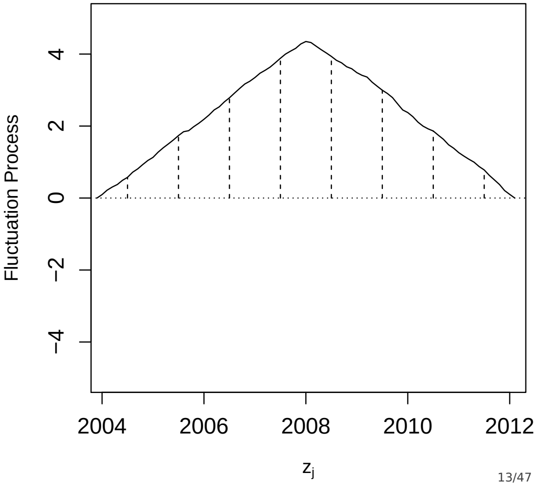
Idea: In many situations, a single global model $\mathcal{M}(y, x, \theta)$ that fits **all** n observations cannot be found. But it might be possible to find a partition w.r.t. the variables $z_1, \dots, z_l$ so that a well-fitting model can be found locally in each cell of the partition.

Tools:

- Assess parameter instability w.r.t to splitting variables z_j $(j = 1, \dots, l)$.
- A general measure of deviation from the model is the score or estimating function $\psi(y, x, \theta)$.

2. Tests for parameter instability





2. Tests for parameter instability

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 $\mathcal{M}(y, x, \widehat{\theta})$ just has to be estimated once. Empirical estimating functions $\psi(y_i, x_i, \widehat{\theta})$ just have to be re-ordered and aggregated for each z_j.

2. Tests for parameter instability

Class of 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 $\sigma(z_{ij})$.

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

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

2. Tests for parameter instability

Splitting numeric variables: Assess instability using supLM statistics.

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

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

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

Potential alternatives: Many other parameter instability tests from the same class of tests, e.g., a Cramér-von Mises test (or Nyblom-Hansen test), MOSUM tests, etc.

2. Tests for parameter instability

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

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

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

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

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

2. Tests for parameter instability

Splitting ordinal variables: Several strategies conceivable. Assess instability either as for categorical variables (if C is low), or as for numeric variables (if C is high), or via a specialized test.

$$
\begin{aligned}
\lambda_{maxLMo}(W_j) &= \max_{i \in \{i_1, \dots, i_{C-1}\}} \left(\frac{i}{n} \cdot \frac{n-i}{n} \right)^{-1} \left\| W_j\left(\frac{i}{n}\right) \right\|_2^2, \\
\lambda_{WDMo}(W_j) &= \max_{i \in \{i_1, \dots, i_{C-1}\}} \left(\frac{i}{n} \cdot \frac{n-i}{n} \right)^{-1/2} \left\| W_j\left(\frac{i}{n}\right) \right\|_\infty.
\end{aligned}
$$

Interpretation: Assess only the possible splitpoints $i_1, \dots, i_{C-1}$, based on L_2 or L_∞ norm.

Limiting distribution: Maximum from selected points in a squared Bessel process or multivariate normal distribution, respectively.

2. Tests for parameter instability

Alternative inference frameworks: Classic association tests for independence of y and z_j can be turned into model-based tests by using model scores $\psi(y, x, \hat{\theta})$ instead of just y (Schlosser, Hothorn, Zeileis 2019, *arXiv*).

2. Tests for parameter instability

Alternative inference frameworks: Classic association tests for independence of y and z_j can be turned into model-based tests by using model scores $\psi(y, x, \hat{\theta})$ instead of just y (Schlosser, Hothorn, Zeileis 2019, *arXiv*).

CTree: Hothorn, Hornik, Zeileis (2006, *JCGS*).

- Based on conditional inference (or permutation tests).
- Originally nonparametric.

2. Tests for parameter instability

Alternative inference frameworks: Classic association tests for independence of y and z_j can be turned into model-based tests by using model scores $\psi(y, x, \hat{\theta})$ instead of just y (Schlosser, Hothorn, Zeileis 2019, *arXiv*).

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- Based on conditional inference (or permutation tests).
- Originally nonparametric.

GUIDE: Loh (2002, *Statistica Sinica*).

- Based on χ^2 tests.
- Originally based on residuals only (not full model scores).
- Categorizes both z_j and the model residuals (or scores) into bins.

3. Splitting

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

$$\sum_b \sum_{i \in I_b} \Psi(y_i, x_i, \theta_b).$$

$B = 2$: 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 splitting. Optionally, $B = C$ can be chosen (without search) for categorical variables.

3. Splitting

Alternatively:

- Selecting the optimal split w.r.t. the objective function $\Psi(y, x, \theta)$ requires refitting the model and may be costly.
- Employ a maximally-selected score-based test statistic instead.
- Avoids refitting the model and is thus much cheaper to compute.

4. Pruning

Goal: Avoid overfitting.

Pre-pruning:

- Internal stopping criterium.
- Stop splitting when there is no significant parameter instability.
- Based on Bonferroni-corrected p values of the parameter instability tests.

Post-pruning:

- Grow large tree (e.g., with high significance level).
- Prune splits that do not improve the model fit based on information criteria (e.g., AIC or BIC).

Hyperparameters: Significance level and information criterion penalty can be chosen manually (or possibly through cross-validation etc.).

Parties, Models, Mobsters

Software

Software

Workhorse function: `mob()` for

- data handling,
- calling model fitters,
- carrying out parameter instability tests and
- recursive partitioning algorithm.

Required functionality:

- *Parties:* Class and methods for recursive partytions.
- *Models:* Model fitting functions (optimizing suitable objective function).
- *Mobsters:* High-level interfaces (`lmtree()`, `glmtree()`, `bttree()`, `...`) that call lower-level `mob()` with suitable options and methods.

Software

Parties: S3 class '`modelparty`' built on '`party`'.

- Separates data and tree structure.
- Inherits generic infrastructure for printing, predicting, plotting, ...

Models: Plain functions with input/output convention.

- Basic and extended interface for rapid prototyping and for speeding up computings, respectively.
- Only minimial glue code required if models are well-designed.

Mobsters:

- `mob()` completely agnostic regarding models employed.
- Separate interfaces `lmtree()`, `glmtree()`, ...
- New interfaces typically need to bring their model fitter and adapt the main methods `print()`, `plot()`, `predict()` etc.

Software

Input: Basic model interface.

```
fit(y, x = NULL, start = NULL, weights = NULL, offset = NULL, ...)
```

`y`, `x`, `weights`, `offset` are (the subset of) the preprocessed data.

Starting values are in `start` and further fitting arguments in `...`.

Output: Fitted model object of class with suitable methods.

- `coef()`: Estimated parameters $\hat{\theta}$.
- `logLik()`: Maximized log-likelihood function $-\sum_i \Psi(y_i, x_i, \hat{\theta})$.
- `estfun()`: Empirical estimating functions $\Psi'(y_i, x_i, \hat{\theta})$.

Software

Input: Extended model interface.

```
fit(y, x = NULL, start = NULL, weights = NULL, offset = NULL, ...,
  estfun = FALSE, object = FALSE)
```

Output: List.

- `coefficients`: Estimated parameters $\hat{\theta}$.
- `objfun`: Minimized objective function $\sum_i \Psi(y_i, x_i, \hat{\theta})$.
- `estfun`: Empirical estimating functions $\Psi'(y_i, x_i, \hat{\theta})$.
  Only needed if `estfun = TRUE`, otherwise optionally `NULL`.
- `object`: A model object (providing further methods).
  Only needed if `object = TRUE`, otherwise optionally `NULL`.

Internally: Extended interface constructed from basic interface if supplied.
Efficiency can be gained through extended approach.

Software

Mobsters:

- Distributions: Parametric, multivariate, circular, transformation (*disttree*, *circtree*, *trtf*).
- Linear and generalized linear models (*partykit*, *palmtree*).
- Linear and generalized linear mixed effects models (*glmertree*).
- Survival models (*partykit*, *model4you*).
- Beta regression (*betareg*).
- Psychometric models: Bradley-Terry, item response theory, multinomial processing trees (*psychotree*).
- Structural equation models (*partykit*, *semtree*).
- Network models (*networktree*).
- Spatial lag models (*lagsarlmtree*).

Parties, Models, Mobsters

Bradley-Terry trees

Bradley-Terry trees

Question: Which of these women is more attractive?

And: How does the answer depend on age, gender, and the familiarity with the associated TV show *Germany’s Next Topmodel*?

Bradley-Terry trees

Data: Paired comparisons of attractiveness.

- *Germany's Next Topmodel 2007* finalists: Barbara, Anni, Hana, Fiona, Mandy, Anja.
- Survey with 192 respondents at Universität Tübingen.
- Available covariates: Gender, age, familiarty with the TV show.
- Familiarity assessed by yes/no questions:
  1. Do you recognize the women?/Do you know the show?
  2. Did you watch it regularly?
  3. Did you watch the final show?/Do you know who won?

Bradley-Terry trees

Model: Bradley-Terry (or Bradley-Terry-Luce) model.

- Standard model for paired comparisons in social sciences.
- Parametrizes probability π_{ij} for preferring object *i* over *j* in terms of corresponding "ability" or "worth" parameters θ_i.

$$
\begin{aligned}
\pi_{ij} &= \frac{\theta_i}{\theta_i + \theta_j} \\
\mathrm{logit}(\pi_{ij}) &= \log(\theta_i) - \log(\theta_j)
\end{aligned}
$$

- Maximum likelihood as a logistic or log-linear GLM.

Bradley-Terry trees

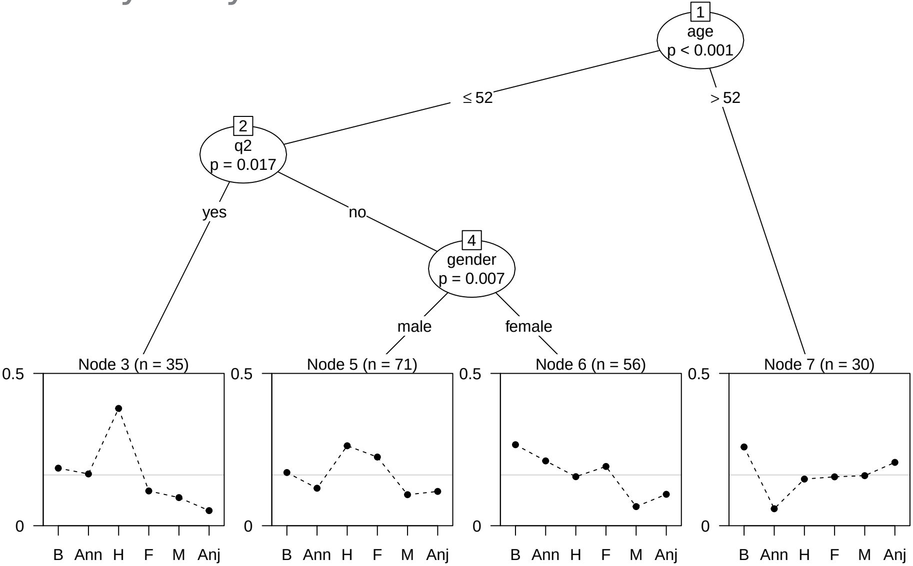
Mobster: Bradley-Terry trees.

- Core infrastructure: Model-fitting function `btmodel()` in *psychotools*.
- High-level interface: `bttree()` in *psychotree*.
- Here: Recreation from scratch using only `mob()` and `btmodel()`.

Illustration:

```
R> library("psychotree")
R> data("Topmodel2007", package = "psychotree")
R> bt <- bttree(preference ~ gender + age + q1 + q2 + q3, data = Topmodel2007)
R> plot(bt)
R> print(bt)
```

Bradley-Terry trees



Bradley-Terry trees

```
Bradley-Terry tree

Model formula:
preference ~ gender + age + q1 + q2 + q3

Fitted party:
[1] root
|   [2] age <= 52
|   |   [3] q2 in yes: n = 35
|   |       Barbara    Anni    Hana   Fiona   Mandy
|   |        1.3378  1.2318  2.0499  0.8339  0.6217
|   |   [4] q2 in no
|   |   |   [5] gender in male: n = 71
|   |   |        Barbara     Anni     Hana    Fiona    Mandy
|   |   |        0.43866  0.08877  0.84629  0.69424 -0.10003
|   |   |   [6] gender in female: n = 56
|   |   |       Barbara    Anni    Hana   Fiona   Mandy
|   |   |        0.9475  0.7246  0.4452  0.6350 -0.4965
|   [7] age > 52: n = 30
|       Barbara    Anni    Hana   Fiona   Mandy
|        0.2178 -1.3166 -0.3059 -0.2591 -0.2357
```

Bradley-Terry trees

```
Number of inner nodes:    3
Number of terminal nodes: 4
Number of parameters per node: 5
Objective function (negative log-likelihood): 1829
```

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```

From scratch: Only need basic model fitting function because `btmodel()` provides all necessary methods.

```
R> btfit1 <- function(y, x = NULL, start = NULL, weights = NULL, offset = NULL, ...) {
+    btmodel(y, weights = weights, ...)
+  }
R> system.time(
+    bt1 <- mob(preference ~ gender + age + q1 + q2 + q3, data = Topmodel2007,
+      fit = btfit1)
+  )

   user  system elapsed 
  4.873   2.879   1.962 
```

Bradley-Terry trees

More efficient: Extended model fitting function.

```
R> btfit2 <- function(y, x = NULL, start = NULL, weights = NULL, offset = NULL, ...,
+    estfun = FALSE, object = FALSE) {
+    rval <- btmodel(y, weights = weights, ..., estfun = estfun, vcov = object)
+    list(
+      coefficients = rval$coefficients,
+      objfun = -rval$loglik,
+      estfun = if(estfun) rval$estfun else NULL,
+      object = if(object) rval else NULL
+    )
+  }
R> system.time(
+    bt2 <- mob(preference ~ gender + age + q1 + q2 + q3, data = Topmodel2007,
+      fit = btfit2)
+  )

   user  system elapsed
  1.407   0.467   1.064
```

Bradley-Terry trees

Infrastructure:

- Basics readily available: `print()`, `plot()`, `predict()`, `coef()`, ...
- Customizable, e.g., model-specific plots, predictions, ...

Here:

```
R> plot(bt2)
R> print(bt2)
```

```
Model-based recursive partitioning (btfit2)

Model formula:
preference ~ gender + age + q1 + q2 + q3
```

Bradley-Terry trees

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Fitted party:
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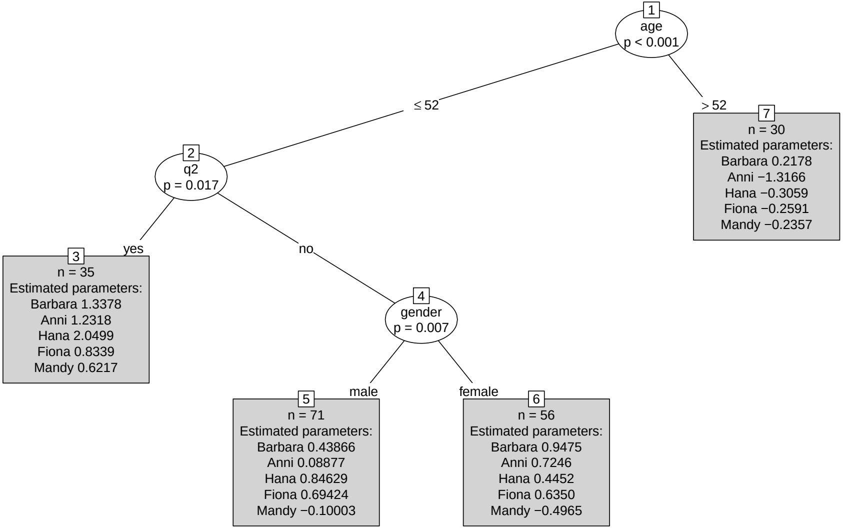

Parties, Models, Mobsters

Model-based random forests

Model-based random forests

Tree:

- *Idea:* Automatic detection of steps and abrupt changes.
- *Goal:* Capture non-linear and non-additive effects and interactions.
- *Result:* Yields B subsamples $\mathcal{B}_b$ with $b = 1, \dots, B$ in which separate local models are estimated.

Model-based random forests

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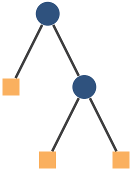
- *Goal:* Capture non-linear and non-additive effects and interactions.
- *Result:* Yields B subsamples $\mathcal{B}_b$ with $b = 1, \dots, B$ in which separate local models are estimated.

Forest:

- *Idea:* Ensemble of T trees based on resampling the learning data.
- *Goal:* Stabilization and regularization, smoother effects.
- *Strategies:* Bootstrap or subsamples. Random input variable sampling.
- *Result:* Yields subsamples $\mathcal{B}_b^t$ with $b = 1, \dots, B^t$ and $t = 1, \dots, T$ for adaptive local model estimation.

Model-based random forests



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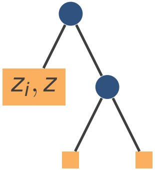
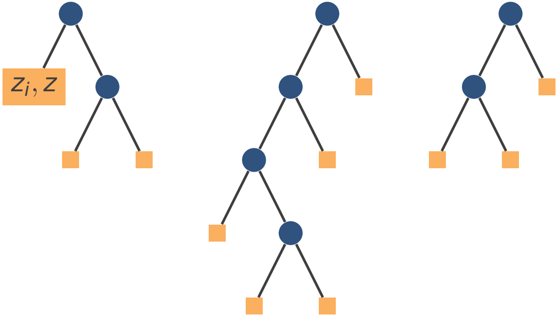


Tree: For predicting a (potentially new) observation z only consider observations corresponding to z_i in the learning data.

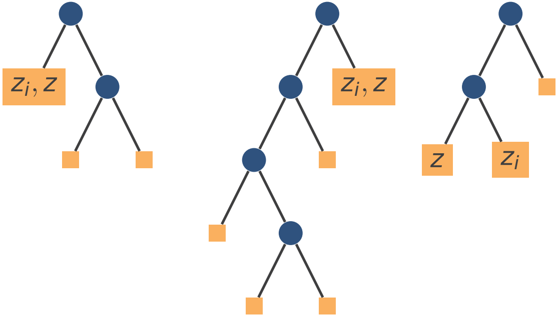
Model-based random forests



Tree: For predicting a (potentially new) observation z only consider observations corresponding to z_i in the learning data.

Forest: Obtain a finer similarity measure between new observation z and z_i.

Model-based random forests



Tree: For predicting a (potentially new) observation z only consider observations corresponding to z_i in the learning data.

Forest: Obtain a finer similarity measure between new observation z and z_i.

Weights: Average over trees, e.g., 2 out of 3 for z_i.

Model-based random forests

Parameter estimator for **a global** model with learning data $\{(y_i, x_i)\}_{i=1,\ldots,n}$:

$$\hat{\theta} = \underset{\theta \in \Theta}{\operatorname{argmin}} \sum_{i=1}^{n} \Psi(y_i, x_i, \theta)$$

Model-based random forests

Parameter estimator for **a global** model with learning data$\{(y_i, x_i, z_i)\}_{i=1,\ldots,n}$:

$$\hat{\theta}(z) = \operatorname*{argmin}_{\theta \in \Theta} \sum_{i=1}^{n} w_i(z) \cdot \Psi(y_i, x_i, \theta)$$

Model-based random forests

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$$\hat{\theta}(z) = \underset{\theta \in \Theta}{\operatorname{argmin}} \sum_{i=1}^{n} w_i(z) \cdot \Psi(y_i, x_i, \theta)$$

Weights:

$$w_i^{\text{base}}(z) \quad = \quad 1$$

Model-based random forests

Parameter estimator for **an adaptive local** model with learning data$\{(y_i, x_i, z_i)\}_{i=1,\ldots,n}$:

$$\hat{\theta}(z) = \underset{\theta \in \Theta}{\operatorname{argmin}} \sum_{i=1}^{n} w_i(z) \cdot \Psi(y_i, x_i, \theta)$$

Weights:

$$\begin{aligned} w_i^{\text{base}}(z) &= 1 \\ w_i^{\text{tree}}(z) &= \sum_{b=1}^{B} I((z_i \in \mathcal{B}_b) \wedge (z \in \mathcal{B}_b)) \end{aligned}$$

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Weights:

$$\begin{aligned}
w_i^{\text{base}}(z) &= 1 \\
w_i^{\text{tree}}(z) &= \sum_{b=1}^{B} I((z_i \in \mathcal{B}_b) \wedge (z \in \mathcal{B}_b)) \\
w_i^{\text{forest}}(z) &= \frac{1}{T} \sum_{t=1}^{T} \sum_{b=1}^{B^t} \frac{I((z_i \in \mathcal{B}_b^t) \wedge (z \in \mathcal{B}_b^t))}{|\mathcal{B}_b^t|}
\end{aligned}$$

Model-based random forests

Software:

- `cforest()` based on `ctree()` in *partykit*.
- Redesign of *partykit* internals in development to facilitate “plug & play” trees and forests.
- `pmforest()` for personalized treatment effects in *model4you*.
- `traforest()` for transformation forests in *trtf*.
- `distforest()` for distributional forests in *disttree* on R-Forge.
- `circforest()` for circular forests in *circtree* on R-Forge.

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