9
Additive Models
&
Trees

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1) Generalized additive models

$$\mathrm{E}(Y|X_1, X_2, \ldots, X_p) = \alpha + f_1(X_1) + f_2(X_2) + \cdots + f_p(X_p)$$

- $X_1, X_2, \ldots, X_p$: predictors
- Y : the outcome
- the f_j's : unspecified smooth ("nonparametric") functions

- we fit each function using a scatterplot smoother
  (e.g., a cubic smoothing spline or kernel smoother)
- provide an algorithm for simultaneously estimating all p functions

2) Fitting Additive Models

- The additive model has the form

$$Y = \alpha + \sum_{j=1}^{p} f_j(X_j) + \varepsilon$$

$$\mathrm{PRSS}(\alpha, f_1, f_2, \ldots, f_p) = \sum_{i=1}^{N}\left(y_i - \alpha - \sum_{j=1}^{p} f_j(x_{ij})\right)^2 + \sum_{j=1}^{p} \lambda_j \int f_j''(t_j)^2 dt_j,$$

,where the $\lambda_j \geq 0$ are tuning parameters

- minimizer of (9.7) is an additive cubic spline model
- each of the functions f_j is a cubic spline in the component Xj , with knots at each of the unique values of xij , i = 1, . . . ,N
- without further restrictions on the model ➡ the solution is not unique

2) Fitting Additive Models

Algorithm 9.1 *The Backfitting Algorithm for Additive Models.*

1. Initialize: $\hat{\alpha} = \frac{1}{N}\sum_1^N y_i,\ \hat{f}_j \equiv 0, \forall i, j.$

2. Cycle: $j = 1, 2, \ldots, p, \ldots, 1, 2, \ldots, p, \ldots,$

$$\hat{f}_j \leftarrow \mathcal{S}_j\left[\{y_i - \hat{\alpha} - \sum_{k \neq j} \hat{f}_k(x_{ik})\}_1^N\right],$$

$$\hat{f}_j \leftarrow \hat{f}_j - \frac{1}{N}\sum_{i=1}^{N} \hat{f}_j(x_{ij}).$$

until the functions $\hat{f}_j$ change less than a prespecified threshold.

3) Additive Logistic Regression

- The generalized additive logistic model has the form

$$\log \frac{\Pr(Y=1|X)}{\Pr(Y=0|X)} = \alpha + f_1(X_1) + \cdots + f_p(X_p).$$

- The functions $f_1, f_2, \ldots, f_p$ are estimated by a backfitting algorithm within a Newton–Raphson procedure

- The additive model fitting in step (2) of Algorithm 9.2 requires a weighted scatterplot smoother.

3) Additive Logistic Regression

Algorithm 9.2 *Local Scoring Algorithm for the Additive Logistic Regression Model.*

1. Compute starting values: $\hat{\alpha} = \log[\bar{y}/(1-\bar{y})]$, where $\bar{y} = \text{ave}(y_i)$, the sample proportion of ones, and set $\hat{f}_j \equiv 0\ \forall j$.

2. Define $\hat{\eta}_i = \hat{\alpha} + \sum_j \hat{f}_j(x_{ij})$ and $\hat{p}_i = 1/[1+\exp(-\hat{\eta}_i)]$.

   Iterate:

   (a) Construct the working target variable

   $$z_i = \hat{\eta}_i + \frac{(y_i - \hat{p}_i)}{\hat{p}_i(1-\hat{p}_i)}.$$

   (b) Construct weights $w_i = \hat{p}_i(1-\hat{p}_i)$

   (c) Fit an additive model to the targets z_i with weights w_i, using a weighted backfitting algorithm. This gives new estimates $\hat{\alpha}, \hat{f}_j,\ \forall j$

3. Continue step 2. until the change in the functions falls below a prespecified threshold.

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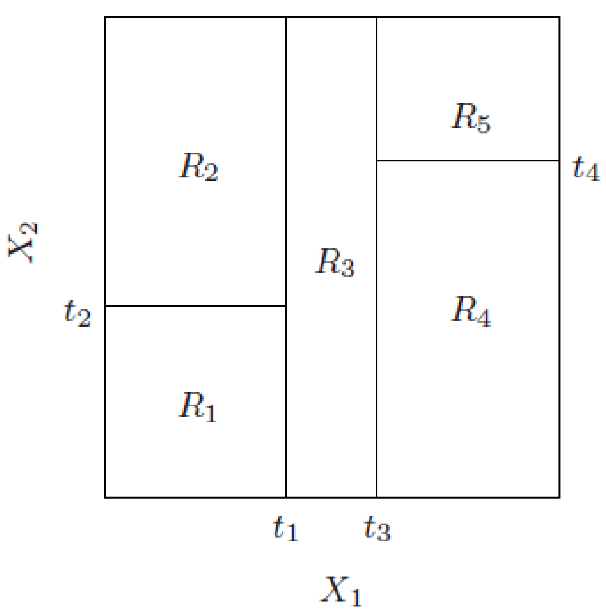
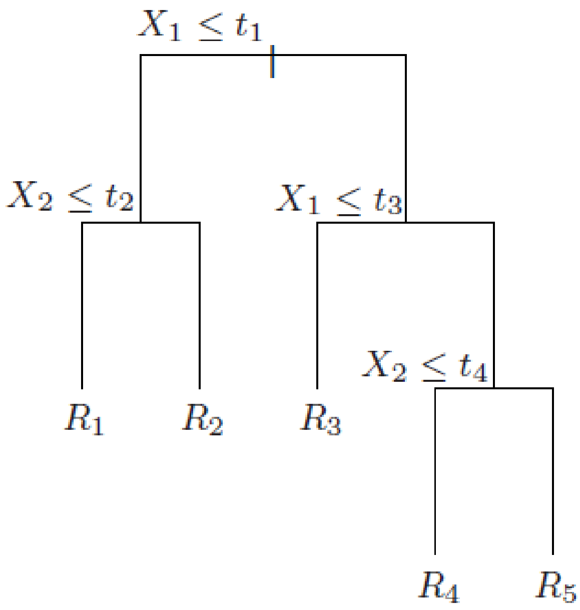
1) Tree-Based Methods

- Tree-based methods partition the feature space into a set of rectangles
- fit a simple model (like a constant) in each one.
- a popular method for tree-based regression and classification called CART





2) Regression Trees

- Suppose first that we have a partition into M regions $R_1, R_2, \ldots, R_M$,
- we model the response as a constant c_m in each region:

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m)$$

- Now finding the best binary partition

$$R_1(j,s) = \{X | X_j \le s\} \text{ and } R_2(j,s) = \{X | X_j > s\}$$

$$\min_{j,\, s} \Big[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2 \Big]$$

$$\Downarrow$$

$$\hat{c}_1 = \text{ave}(y_i | x_i \in R_1(j,s)) \text{ and } \hat{c}_2 = \text{ave}(y_i | x_i \in R_2(j,s))$$

2) Regression Trees

- How large should we grow the tree?

  a very large tree might overfit the data
  a small tree might not capture the important structure

- *cost-complexity pruning*

  Find tree which minimizes

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha|T|$$

$$N_m = \#\{x_i \in R_m\},$$

$$\hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i,$$

$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2$$

- Choosing α adaptively by weakest link pruning

- α the tradeoff between tree size and its goodness of fit to the dat

3) Classification Trees

- Only change in the criteria to split nodes and pruning the tree
- $\hat{p}_{mk}$: proportion of class k on node m

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k),$$

- k(m) be the majority class on node m, i.e. $k(m) = \arg\max_k \hat{p}_{mk}$;

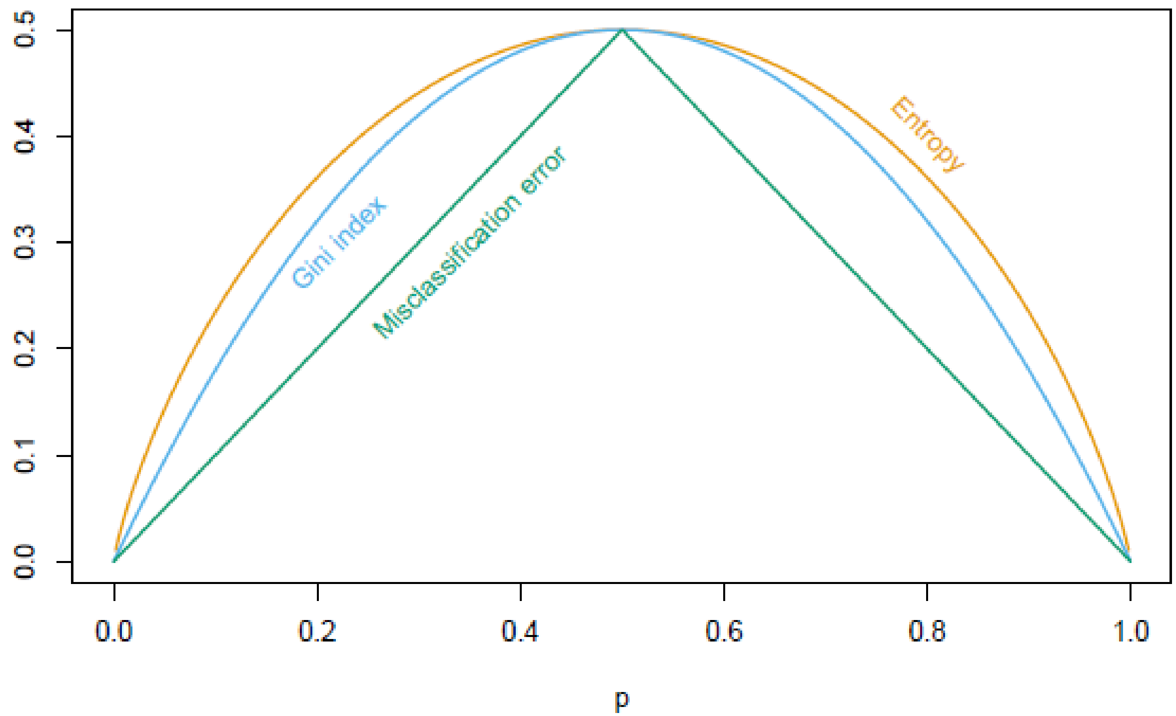
- For each node, partition to minimize

Misclassification error: $\frac{1}{N_m} \sum_{i \in R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{mk(m)}$.

Gini index: $\sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$.

Cross-entropy or deviance: $-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$.

3) Classification Trees



- Cross-entropy and Gini index are more sensitive to changes in the node probabilities than the misclassification rate.
- Either cross-entropy and Gini index should be used when growing the tree.

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THANK YOU