Statistics and learning

Learning Decision Trees and an Introduction to Boosting

Emmanuel Rachelson and Matthieu Vignes

ISAE SupAero

Friday 15th March 2013

Keywords

- Decision trees
- Divide and Conquer
- Impurity measure, Gini index, Information gain
- Pruning and overfitting
- CART and C4.5

Contents of this class:

The general idea of learning decision trees

Regression trees

Classification trees

Boosting and trees

Introductory example

	Alt	Bar	F/S	Hun	Pat	Pri	Rai	Res	Typ	Dur	Wai
x_1	Y	N	N	Y	0.38	$$$	N	Y	French	8	Y
x_2	Y	N	N	Y	0.83	$	N	N	Thai	41	N
x_3	N	Y	N	N	0.12	$	N	N	Burger	4	Y
x_4	Y	N	Y	Y	0.75	$	Y	N	Thai	12	Y
x_5	Y	N	Y	N	0.91	$$$	N	Y	French	75	N
x_6	N	Y	N	Y	0.34	$$	Y	Y	Italian	8	Y
x_7	N	Y	N	N	0.09	$	Y	N	Burger	7	N
x_8	N	N	N	Y	0.15	$$	Y	Y	Thai	10	Y
x_9	N	Y	Y	N	0.84	$	Y	N	Burger	80	N
x_{10}	Y	Y	Y	Y	0.78	$$$	N	Y	Italian	25	N
x_{11}	N	N	N	N	0.05	$	N	N	Thai	3	N
x_{12}	Y	Y	Y	Y	0.89	$	N	N	Burger	38	Y

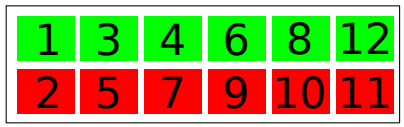
Please describe this dataset *without* any calculation.

Introductory example

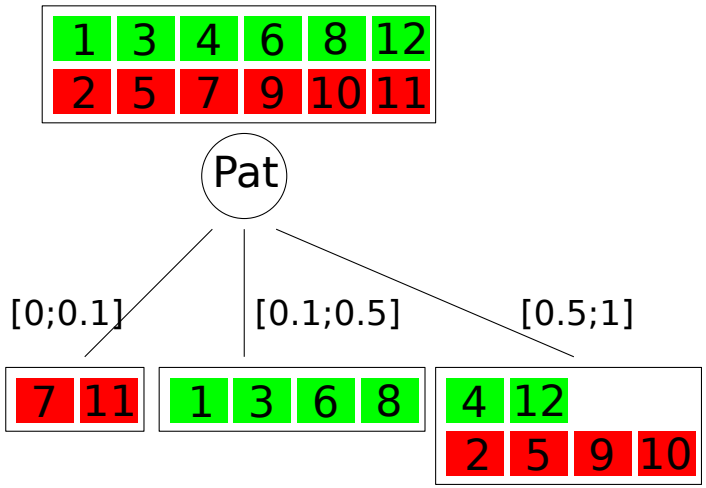
	Alt	Bar	F/S	Hun	Pat	Pri	Rai	Res	Typ	Dur	Wai
x_1	Y	N	N	Y	0.38	$$$	N	Y	French	8	Y
x_2	Y	N	N	Y	0.83	$	N	N	Thai	41	N
x_3	N	Y	N	N	0.12	$	N	N	Burger	4	Y
x_4	Y	N	Y	Y	0.75	$	Y	N	Thai	12	Y
x_5	Y	N	Y	N	0.91	$$$	N	Y	French	75	N
x_6	N	Y	N	Y	0.34	$$	Y	Y	Italian	8	Y
x_7	N	Y	N	N	0.09	$	Y	N	Burger	7	N
x_8	N	N	N	Y	0.15	$$	Y	Y	Thai	10	Y
x_9	N	Y	Y	N	0.84	$	Y	N	Burger	80	N
x_{10}	Y	Y	Y	Y	0.78	$$$	N	Y	Italian	25	N
x_{11}	N	N	N	N	0.05	$	N	N	Thai	3	N
x_{12}	Y	Y	Y	Y	0.89	$	N	N	Burger	38	Y

Why is Pat a better indicator than Typ?

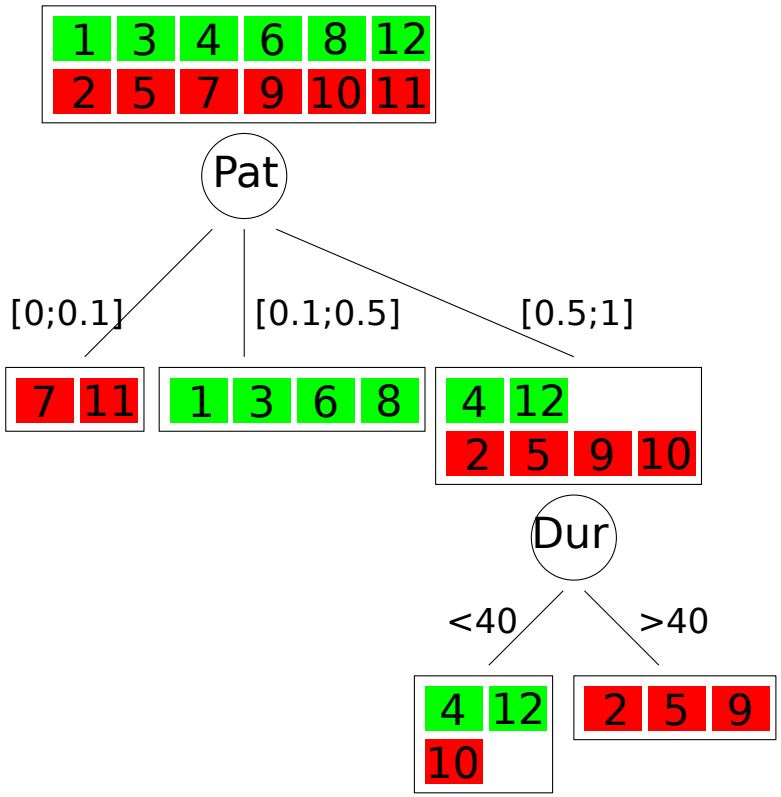
Deciding to wait. . . or not



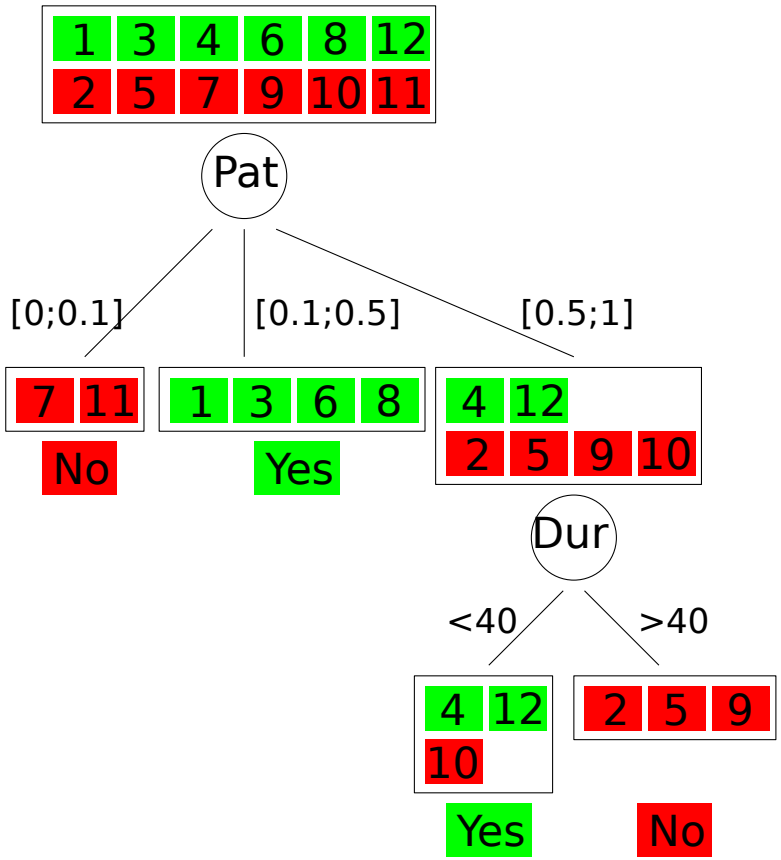
Deciding to wait. . . or not



Deciding to wait. . . or not



Deciding to wait. . . or not



Decision trees

Ingredients:

- Nodes
  Each node contains a *test* on the features which *partitions* the data.
- Edges
  The outcome of a node's test leads to one of its child edges.
- Leaves
  A terminal node, or leaf, holds a *decision value* for the output variable.

Decision trees

Ingredients:

- Nodes
  Each node contains a *test* on the features which *partitions* the data.
- Edges
  The outcome of a node's test leads to one of its child edges.
- Leaves
  A terminal node, or leaf, holds a *decision value* for the output variable.

We will look at binary trees ($\Rightarrow$ binary tests) and single variable tests.

Binary attribute:	node = attribute
Continuous attribute:	node = (attribute, threshold)

Decision trees

Ingredients:

- Nodes
  Each node contains a *test* on the features which *partitions* the data.
- Edges
  The outcome of a node's test leads to one of its child edges.
- Leaves
  A terminal node, or leaf, holds a *decision value* for the output variable.

We will look at binary trees ($\Rightarrow$ binary tests) and single variable tests.

Binary attribute:	node = attribute
Continuous attribute:	node = (attribute, threshold)

How does one build a good decision tree?
For a regression problem?
For a classification problem?

A little more formally

A tree with M leaves describes a covering set of M hypercubes R_m in X. Each R_m hold a decision value $\hat{y}_m$.

$$\hat{f}(x) = \sum_{m=1}^{M} \hat{y}_m I_{R_m}(x)$$

Notation:

$$N_m = |x_i \in R_m| = \sum_{i=1}^{q} I_{R_m}(x_i)$$

The general idea: divide and conquer

Example Set T, attributes $x_1, \ldots, x_p$
FormTree(T)

1. Find best split (j, s) over T // Which criterion?
2. If $(j, s) = \emptyset$,
   - node = FormLeaf(T) // Which value for the leaf?
3. Else
   - node $= (j, s)$
   - split T according to (j, s) into $(T1, T2)$
   - append FormTree($T1$) to node // Recursive call
   - append FormTree($T2$) to node
4. Return node

The general idea: divide and conquer

Example Set T, attributes $x_1, \ldots, x_p$
FormTree(T)

1. Find best split (j, s) over T // Which criterion?
2. If $(j, s) = \emptyset$,
   - node = FormLeaf(T) // Which value for the leaf?
3. Else
   - node $= (j, s)$
   - split T according to (j, s) into $(T1, T2)$
   - append FormTree($T1$) to node // Recursive call
   - append FormTree($T2$) to node
4. Return node

Remark

This is a greedy algorithm, performing local search.

The R point of view

Two packages for tree-based methods: `tree` and `rpart`.

Regression trees – criterion

We want to fit a tree to the data $\{(x_i, y_i)\}_{i=1..q}$ with $y_i \in \mathbb{R}$.

Criterion?

Regression trees – criterion

We want to fit a tree to the data $\{(x_i, y_i)\}_{i=1..q}$ with $y_i \in \mathbb{R}$.

Criterion? Sum of squares: $\sum_{i=1}^{q} \left(y_i - \hat{f}(x_i) \right)^2$

Regression trees – criterion

We want to fit a tree to the data $\{(x_i, y_i)\}_{i=1..q}$ with $y_i \in \mathbb{R}$.

Criterion? Sum of squares: $\sum_{i=1}^{q} \left(y_i - \hat{f}(x_i) \right)^2$

Inside region R_m, best $\hat{y}_m$?

Regression trees – criterion

We want to fit a tree to the data $\{(x_i, y_i)\}_{i=1..q}$ with $y_i \in \mathbb{R}$.

Criterion? Sum of squares: $\sum_{i=1}^{q} \left(y_i - \hat{f}(x_i) \right)^2$

Inside region R_m, best $\hat{y}_m$? $\hat{y}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i = \overline{Y}_{R_m}$

Node impurity measure:

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

Regression trees – criterion

Best partition: hard to find. But locally, best split?

Regression trees – criterion

Best partition: hard to find. But locally, best split? Solve $\underset{j,s}{\operatorname{argmin}} C(j,s)$

$$
\begin{aligned}
C(j,s) &= \left[\min_{\hat{y}_1} \sum_{x_i \in R_1(j,s)} (y_i - \hat{y}_1)^2 + \min_{\hat{y}_2} \sum_{x_i \in R_2(j,s)} (y_i - \hat{y}_2)^2 \right] \\
&= \left[\sum_{x_i \in R_1(j,s)} \left(y_i - \overline{Y}_{R_1(j,s)}\right)^2 + \sum_{x_i \in R_1(j,s)} \left(y_i - \overline{Y}_{R_2(j,s)}\right)^2 \right] \\
&= N_1 Q_1 + N_2 Q_2
\end{aligned}
$$

Overgrowing the tree?

- Too small: rough average.
- Too large: overfitting.

	Alt	Bar	F/S	Hun	Pat	Pri	Rai	Res	Typ	Dur
x_1	Y	N	N	Y	0.38	$$$	N	Y	French	8
x_2	Y	N	N	Y	0.83	$	N	N	Thai	41
x_3	N	Y	N	N	0.12	$	N	N	Burger	4
x_4	Y	N	Y	Y	0.75	$	Y	N	Thai	12
x_5	Y	N	Y	N	0.91	$$$	N	Y	French	75
x_6	N	Y	N	Y	0.34	$$	Y	Y	Italian	8
x_7	N	Y	N	N	0.09	$	Y	N	Burger	7
x_8	N	N	N	Y	0.15	$$	Y	Y	Thai	10
x_9	N	Y	Y	N	0.84	$	Y	N	Burger	80
x_{10}	Y	Y	Y	Y	0.78	$$$	N	Y	Italian	25
x_{11}	N	N	N	N	0.05	$	N	N	Thai	3
x_{12}	Y	Y	Y	Y	0.89	$	N	N	Burger	38

Overgrowing the tree?

Stopping criterion?

- Stop if $\min_{j,s} C(j,s) > \kappa$? Not good because a good split might be hidden in deeper nodes.
- Stop if $N_m < n$? Good to avoid overspecialization.
- Prune the tree after growing. *cost-complexity pruning*.

Cost-complexity criterion:

$$C_\alpha = \sum_{m=1}^{M} N_m Q_m + \alpha M$$

Once a tree is grown, prune it to minimize C_α.

- Each α corresponds to a unique cost-complexity optimal tree.
- Pruning method: *Weakest link pruning*, left to your curiosity.
- Best α? Through cross-validation.

Regression trees in a nutshell

- Constant values on the leaves.
- Growing phase: greedy splits that minimize the squared-error impurity measure.
- Pruning phase: Weakest-link pruning that minimize the cost-complexity criterion.

Regression trees in a nutshell

- Constant values on the leaves.
- Growing phase: greedy splits that minimize the squared-error impurity measure.
- Pruning phase: Weakest-link pruning that minimize the cost-complexity criterion.

Further reading on regression trees:

- MARS: Multivariate Adaptive Regression Splines.
  Linear functions on the leaves.
- PRIM: Patient Rule Induction Method.
  Focuses on extremas rather than averages.

A bit of R before classification tasks

Let's load the "Optical Recognition of Handwritten Digits" database.

```
> optical <- read.csv("optdigits.tra", sep=",",
header=FALSE)
> colnames(optical)[65] <- "class"
```

Classification trees

Suppose $y_i \in \{True; False\}$. Let's fit a tree to $\{(x_i, y_i)\}_{i=1..q}$.

Best $\hat{y}_m$ in node m ?

Classification trees

Suppose $y_i \in \{True; False\}$. Let's fit a tree to $\{(x_i, y_i)\}_{i=1..q}$.

Best $\hat{y}_m$ in node m ?
Proportion of class k observations in node m:

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

Class of node m: $\hat{y}_m = \underset{k}{\operatorname{argmax}}\, \hat{p}_{mk}$

Classification trees

Node impurity measure?

Misclassification error $$Q_m = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i \neq \hat{y}_m) = 1 - \hat{p}_{m\hat{y}_m}$$

Gini index (CART) $$Q_m = \sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk} \left(1 - \hat{p}_{mk}\right)$$

Information or deviance (C4.5) $$Q_m = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

Classification trees

Node impurity measure?

Misclassification error $$Q_m = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i \neq \hat{y}_m) = 1 - \hat{p}_{m\hat{y}_m}$$

Gini index (CART) $$Q_m = \sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk} \left(1 - \hat{p}_{mk}\right)$$

Information or deviance (C4.5) $$Q_m = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

Splitting criterion? Minimize $N_1 Q_1 + N_2 Q_2$

Classification trees

Node impurity measure?

Misclassification error $$Q_m = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i \neq \hat{y}_m) = 1 - \hat{p}_{m\hat{y}_m}$$

Gini index (CART) $$Q_m = \sum_{k \neq k'} \hat{p}_{mk}\hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}\left(1 - \hat{p}_{mk}\right)$$

Information or deviance (C4.5) $$Q_m = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

Splitting criterion? Minimize $N_1 Q_1 + N_2 Q_2$

Pruning? Cost-complexity (often using the misclassification error) criterion.

$$C_\alpha = \sum_{m=1}^{M} N_m Q_m + \alpha M$$

Classification trees in a nutshell

- Class values on the leaves.
- Growing phase: greedy splits that maximize the Gini index reduction (CART) or the information gain (C4.5)
- Pruning phase: Weakest-link pruning that minimize the cost-complexity criterion.

Classification trees in a nutshell

- Class values on the leaves.
- Growing phase: greedy splits that maximize the Gini index reduction (CART) or the information gain (C4.5)
- Pruning phase: Weakest-link pruning that minimize the cost-complexity criterion.

Further reading on classification trees:

- EC4.5 and YaDT: Implementation improvements for C4.5
- C5.0: C4.5 with additional features.
- Loss matrix.
- Handling missing values.

A bit of R

```
> help(tree)
> optical.tree <- tree(factor(class) ~., optical,
split="deviance")
> optical.tree.gini <- tree(factor(class) ~., optical,
split="gini")
> plot(optical.tree); text(optical.tree)
> help(prune.tree)
> optical.tree.pruned <- prune.tree(optical.tree,
method="misclass", k=10)
> help(cv.tree)
> optical.tree.cv <- cv.tree(optical.tree, ,
prune.misclass)
> plot(optical.tree.cv)
```

Why should you use Decision Trees?

Advantages

- Easy to read and interpret.
- Learning the tree has complexity linear in p.
- Can be rather efficient on well pre-processed data (in conjunction with PCA for instance).

However

- No margin or performance guarantees.
- Lack of smoothness in the regression case.
- Strong assumption that the data can fit in hypercubes.
- Strong sensitivity to the data set.

But...

- Can be compensated by ensemble methods such as Boosting or Bagging.
- Very efficient extension with Random Forests

Boosting and trees

Motivation

AdaBoost with trees is the best off-the-shelf classifier in the world. (Breiman 1998)

Not so true today but still accurate enough.

What is Boosting?

Key idea

Boosting is a procedure that combines several "weak" classifiers into a powerful "commitee".

Commitee-based or ensemble methods literature in Machine Learning.

Most popular boosting alg. (Freund & Schapire, 1997): AdaBoost.M1.

Warning

For this part, we take a very practical approach. For a more thorough and rigorous presentation, see (for instance) the reference below.

R. E. Schapire. **The boosting approach to machine learning: An overview.** Nonlinear Estimation and Classification, 2002.

The main picture

Weak classifiers

$h(x) = y$ is said to be a *weak* (or a PAC-weak) classifier if it performs better than a random guessing on the training data.

AdaBoost

AdaBoost constructs a strong classifier as a linear combination of weak classifiers $h_t(x)$:

$$f(x) = \sum_{t=1}^{T} \alpha_t h_t(x)$$

The AdaBoost algorithm

Given $\{(x_i, y_i)\}, x_i \in X, y_i \in \{-1; 1\}$.

The AdaBoost algorithm

Given $\{(x_i, y_i)\}, x_i \in X, y_i \in \{-1; 1\}$.
Initialize weights $D_1(i) = 1/q$

The AdaBoost algorithm

Given $\{(x_i, y_i)\}, x_i \in X, y_i \in \{-1; 1\}$.
Initialize weights $D_1(i) = 1/q$
For $t = 1$ to T:

- Find $h_t = \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{q} D_t(i) I(y_i \neq h(x_i))$

The AdaBoost algorithm

Given $\{(x_i, y_i)\}, x_i \in X, y_i \in \{-1; 1\}$.
Initialize weights $D_1(i) = 1/q$
For $t = 1$ to T:

- Find $h_t = \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{q} D_t(i) I(y_i \neq h(x_i))$
- If $\epsilon_t = \sum_{i=1}^{q} D_t(i) I(y_i \neq h_t(x_i)) \geq 1/2$ then stop

The AdaBoost algorithm

Given $\{(x_i, y_i)\}, x_i \in X, y_i \in \{-1; 1\}$.
Initialize weights $D_1(i) = 1/q$
For $t = 1$ to T:

- Find $h_t = \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{q} D_t(i) I(y_i \neq h(x_i))$
- If $\epsilon_t = \sum_{i=1}^{q} D_t(i) I(y_i \neq h_t(x_i)) \geq 1/2$ then stop
- Set $\alpha_t = \frac{1}{2} \log\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$

The AdaBoost algorithm

Given $\{(x_i, y_i)\}, x_i \in X, y_i \in \{-1; 1\}$.
Initialize weights $D_1(i) = 1/q$
For $t = 1$ to T:

- Find $h_t = \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{q} D_t(i) I(y_i \neq h(x_i))$
- If $\epsilon_t = \sum_{i=1}^{q} D_t(i) I(y_i \neq h_t(x_i)) \geq 1/2$ then stop
- Set $\alpha_t = \frac{1}{2} \log\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$
- Update

$$D_{t+1}(i) = \frac{D_t(i) e^{-\alpha_t y_i h_t(x_i)}}{Z_t}$$

Where Z_t is a normalisation factor.

The AdaBoost algorithm

Given $\{(x_i, y_i)\}, x_i \in X, y_i \in \{-1; 1\}$.
Initialize weights $D_1(i) = 1/q$
For $t = 1$ to T:

- Find $h_t = \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{q} D_t(i) I(y_i \neq h(x_i))$
- If $\epsilon_t = \sum_{i=1}^{q} D_t(i) I(y_i \neq h_t(x_i)) \geq 1/2$ then stop
- Set $\alpha_t = \frac{1}{2} \log\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$
- Update

$$D_{t+1}(i) = \frac{D_t(i) e^{-\alpha_t y_i h_t(x_i)}}{Z_t}$$

  Where Z_t is a normalisation factor.

Return the classifier

$$H(x) = sign\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

Iterative reweighting

$$D_{t+1}(i) = \frac{D_t(i) e^{-\alpha_t y_i h_t(x_i)}}{Z_t}$$

- Increase the weight of incorrectly classified samples
- Decrease the weight of correctly classified samples
- Memory effect: a sample misclassified several times has a large $D(i)$
- h_t focusses on samples that were misclassified by $h_0, \ldots, h_{t-1}$

Properties

$$\frac{1}{q}\sum_{i=1}^{q} I\left(H(x_i) \neq y_i\right) \leq \prod_{t=1}^{T} Z_t$$

- To minimize training error at each step t, minimize this upper bound.
  $\rightarrow$ This is where $\alpha_t = \frac{1}{2}\log\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$ comes from.
- This is equivalent to maximizing the margin!

AdaBoost is not Boosting

Many variants of AdaBoost:

- Binary classification AdaBoost.M1, AdaBoost.M2, . . . ,
- Multiclass AdaBoost.MH,
- Regression AdaBoost.R,
- Online, . . .

And other Boosting algorithms.

Why should you use Boosting?

AdaBoost is a meta-algorithm: it "boosts" a weak classif. algorithm into a commitee that is a strong classifier.

- AdaBoost maximizes margin
- Very simple to implement
- Can be seen as a feature selection algorithm
- In practice, AdaBoost often avoids overfitting.

AdaBoost with trees

Your turn to play: will you be able to implement AdaBoost with trees in R?