Decision Trees

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Outline

Trees and decision trees

Growing a tree

Pruning a tree

Machine learning

Supervised learning

- given a data set $\mathcal{D} = ((\mathbf{X}_i, \mathbf{Y}_i))_{1 \leq i \leq N}$
- an algorithm builds a program that maps inputs to desired outputs

A simple example

	Color	Size	Action	Age	Class
1	YELLOW	SMALL	STRETCH	ADULT	TRUE
2	YELLOW	SMALL	STRETCH	CHILD	TRUE
3	YELLOW	SMALL	DIP	ADULT	TRUE
4	YELLOW	SMALL	DIP	CHILD	TRUE
5	YELLOW	LARGE	STRETCH	ADULT	TRUE
6	YELLOW	LARGE	STRETCH	CHILD	FALSE
7	YELLOW	LARGE	DIP	ADULT	FALSE
8	YELLOW	LARGE	DIP	CHILD	FALSE
9	PURPLE	SMALL	STRETCH	ADULT	TRUE
10	PURPLE	SMALL	STRETCH	CHILD	FALSE
11	PURPLE	SMALL	DIP	ADULT	FALSE
12	PURPLE	SMALL	DIP	CHILD	FALSE
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14	PURPLE	LARGE	STRETCH	CHILD	FALSE
15	PURPLE	LARGE	DIP	ADULT	FALSE
16	PURPLE	LARGE	DIP	CHILD	FALSE

Perfect solution

```
function CLASS(Color, Size, Action, Age)
    if Color=Yellow and Size=Small then
        return True
    else
        if Action=Stretch and Age=Adult then
            return True
        else
            return False
        end if
    end if
end function
```

Simplified programs

In this example

- a series of tests (questions)
- each test consists in matching the value of a variable with a target value
- could be rewritten to get rid of the `and` operator
- in many cases no loops are required

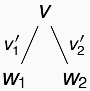
Building programs

- use this simple representation for machine learning
- build a model as a series of tests followed by a “decision”

Tree based representation

Trees

- numerous (equivalent) mathematical definitions
- simple recursive one: a tree consists in a value v and a possibly empty list of trees, each named by a value v' (they are *sub-trees*)
- examples:
  - $(v, \emptyset)$, simplified into v
  - $(v, ((v'_1, (w_1, \emptyset)), (v'_2, (w_2, \emptyset))))$, simplified into $(v, v'_1 \Rightarrow w_1, v'_2 \Rightarrow w_2)$ or better into

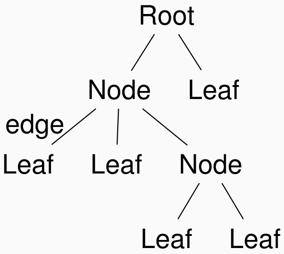


- notice that labelling the sub-trees is application specific (many do not use such labels)

Vocabulary

- each tree consists of a root node and of possibly sub-trees
- a tree without sub-trees is a leaf
- the root node of a sub-tree in a larger tree is simple called a node
- an edge materializes the connection between a tree and a sub-tree and is labelled by the name of the sub-tree

a tree of height 3



- a branch is a series of edges going down the tree
- the height of a tree is the number of edges of its longest branch

Decision trees

Informal definition

A decision tree is a simplified program represented by a tree in which a series of tests are conducted against an input. Each test is represented by a node. Edges correspond to test results and leaves to outputs (a.k.a. decisions).

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```
if Age=Child then
    return False
else
    return True
end if
```

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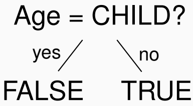


Age = CHILD?

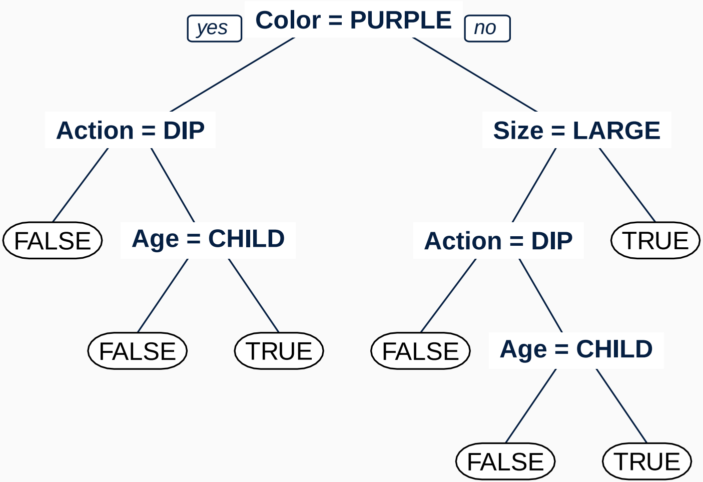
yes

no

FALSE

TRUE

A more complex example



Decision trees

Standard data spaces

- $\mathcal{X}$: input space ($\mathbf{X} \in \mathcal{X}$)
- $\mathcal{Y}$: output space ($\mathbf{Y} \in \mathcal{Y}$)

Definition

A decision tree on $\mathcal{X} \times \mathcal{Y}$ is a tree such that:

- each node n is associated to a function f_n from $\mathcal{X}$ to $\mathcal{O}_n$ a finite set
- a node n has exactly $|\mathcal{O}_n|$ sub-trees with labelled with distinct elements of $\mathcal{O}_n$
- each leaf's value is an element of $\mathcal{Y}$

$\mathcal{T}(\mathcal{X}, \mathcal{Y})$: the set of all decision trees on $\mathcal{X} \times \mathcal{Y}$.

Taking decisions

Using a decision tree

- a decision tree T implements a function g_T from $\mathcal{X}$ to $\mathcal{Y}$
- given $\mathbf{x}$, one navigates from the top of the tree to a leaf, according to test results
- $g_T(\mathbf{x})$ is the value associated to the leaf

Formal definition

$g_T(\mathbf{x})$ is given by:

- $\mathbf{y}$ if $T = \mathbf{y}$ (a tree which consists in a single leaf with value $\mathbf{y}$)
- $g_{T_l}(\mathbf{x})$ if $T = (f_n, (o_1, T_1), \ldots, (o_k, T_k))$ where $o_l = f_n(\mathbf{x})$. Indeed in this case
  - T has for value the function f_n and has as many sub-trees as possible outputs of f_n
  - then T_l is the sub-tree associated $f_n(\mathbf{x})$

Data model

Multivariate assumption

$\mathcal{X}$ is structured into “variables”:

- $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2 \times \ldots \times \mathcal{X}_P$
- $\mathbf{X} = (X_1, X_2, \ldots, X_P)^T$
- $\mathbf{x} = (x_1, x_2, \ldots, x_P)^T$
- the test in a decision tree node operates only on one variable

Variable types

- $\mathcal{X}_k$ is either $\mathbb{R}$ or finite
- different variables can have different types (mixed data)
- $\mathcal{Y}$ is also either $\mathbb{R}$ or finite

Tests

Trivial tests

- $f_n(\mathbf{x}) = x_j$
- only when $|\mathcal{X}_j| < \infty$
- ID3/C4.5 algorithms (Quinlan)

Binary tests

- 1/0, yes/no, true/false output
- $f_n(\mathbf{x}) = \mathbf{1}_{x_j \in A}$ with $A \subset \mathcal{X}_j$ when $|\mathcal{X}_j| < \infty$
- $f_n(\mathbf{x}) = \mathbf{1}_{x_j \leq \lambda}$ when $\mathcal{X}_j = \mathbb{R}$
- CART (Breiman et al.)

Building a decision tree

Supervised learning

- given a data set $\mathcal{D} = ((\mathbf{X}_i, \mathbf{Y}_i))_{1 \leq i \leq N}$ and a loss function l
- how to build a tree T such that $R_l(g_T)$ is as small as possible?

Key idea

Recursively grow the tree

- split the data set into sub data-sets based on a test
- recursively apply a tree growing algorithm on each sub-set
- join the sub-trees into a tree with the test at its root

Outline

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Pruning a tree

Optimal leaf

Single leaf tree

- if $T = \mathbf{v}$, then $g_T(\mathbf{x}) = \mathbf{v}$ for all $\mathbf{x}$
- then
$$\widehat{R}_l(g_T, \mathcal{D}) = \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} l(\mathbf{v}, \mathbf{y})$$
- easy to solve for $\widehat{\mathbf{y}}^*_l(\mathcal{D})$ that minimizes $\widehat{R}_l(g_T, \mathcal{D})$

Examples

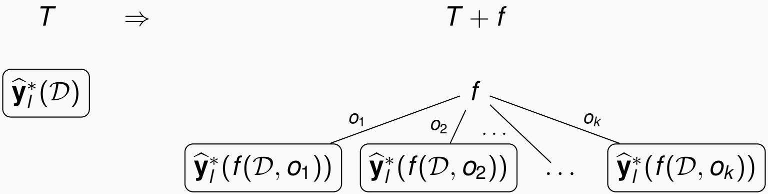
- $\widehat{\mathbf{y}}^*_{l_2}(\mathcal{D}) = \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} \mathbf{y}$ when $l_2(p, v) = (p - v)^2$
- $\widehat{\mathbf{y}}^*_{l_b}(\mathcal{D}) = \arg\max_{\mathbf{y}'\in\mathcal{Y}} |\{(\mathbf{x}, \mathbf{y}) \in \mathcal{D} \mid \mathbf{y} = \mathbf{y}'\}|$ when $l_b(p, v) = \mathbf{1}_{p\neq v}$

Data splitting

Test effects

- a test function f splits a data set into sub-data sets based on $f(\mathbf{X}_i)$
- notation $f(\mathcal{D}, o) = \{(\mathbf{x}, \mathbf{y}) \in \mathcal{D} \mid f(\mathbf{x}) = o\}$
- if f is the test at the root of tree T, then for each $\mathbf{x} \in f(\mathcal{D}, o)$, $g_T(\mathbf{x})$ is computed by the sub-tree associated to o

Tree growing operation



T $\Rightarrow$ $T + f$

$\boxed{\widehat{\mathbf{y}}_l^*(\mathcal{D})}$

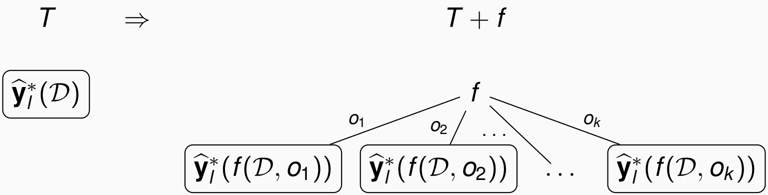
f

o_1 o_2 $\dots$ o_k

$\boxed{\widehat{\mathbf{y}}_l^*(f(\mathcal{D}, o_1))}$ $\boxed{\widehat{\mathbf{y}}_l^*(f(\mathcal{D}, o_2))}$ $\dots$ $\boxed{\widehat{\mathbf{y}}_l^*(f(\mathcal{D}, o_k))}$

Data splitting

Tree growing operation



$T \quad \Rightarrow \quad T+f$

$\boxed{\widehat{\mathbf{y}}_l^*(\mathcal{D})}$

f

o_1

o_2

$\dots$

o_k

$\boxed{\widehat{\mathbf{y}}_l^*(f(\mathcal{D},o_1))}$ $\boxed{\widehat{\mathbf{y}}_l^*(f(\mathcal{D},o_2))}$ $\dots$ $\boxed{\widehat{\mathbf{y}}_l^*(f(\mathcal{D},o_k))}$

- optimal growing for a given f
- empirical risk improvement

$$\widehat{R}_l(g_T,\mathcal{D}) - \widehat{R}_l(g_{T+f},\mathcal{D}) = \frac{1}{|\mathcal{D}|}\sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} \left(l(\widehat{\mathbf{y}}_l^*(\mathcal{D}),\mathbf{y}) - l(\widehat{\mathbf{y}}_l^*(f(\mathcal{D},f(\mathbf{x}))),\mathbf{y})\right)$$

Judging a test/split

General principle

- is $T + f$ better than $T + f'$?
- empirical risk minimization:

$$T + f \text{ is better than } T + f' \Leftrightarrow \widehat{R}_l(g_{T+f}, \mathcal{D}) < \widehat{R}_l(g_{T+f'}, \mathcal{D})$$

Impurity measures

- when $|\mathcal{Y}| < \infty$ impurity measures are more adapted than risk based ones
- notation: $\widehat{p}(\mathbf{y}', \mathcal{D}) = \frac{1}{|\mathcal{D}|} \left|\{(\mathbf{x}, \mathbf{y}) \in \mathcal{D} \mid \mathbf{y} = \mathbf{y}'\}\right|$
- entropy: $\widehat{H}(\mathcal{D}) = -\sum_{\mathbf{y}\in\mathcal{Y}} \widehat{p}(\mathbf{y}, \mathcal{D}) \log \widehat{p}(\mathbf{y}, \mathcal{D})$
- Gini impurity: $I_G(\mathcal{D}) = \sum_{\mathbf{y}\in\mathcal{Y}} \sum_{\mathbf{y}'\in\mathcal{Y}\setminus\{\mathbf{y}\}} \widehat{p}(\mathbf{y}, \mathcal{D})\widehat{p}(\mathbf{y}', \mathcal{D})$

Impurity reduction

Definition

if $\mathcal{I}$ is an impurity measure, the impurity reduction induced by f is

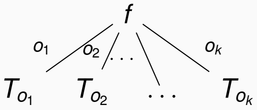
$$\Delta\mathcal{I}(f, \mathcal{D}) = \mathcal{I}(\mathcal{D}) - \sum_{o \in \mathcal{O}} \frac{|f(\mathcal{D}, o)|}{|\mathcal{D}|} \mathcal{I}(f(\mathcal{D}, o))$$

Remarks

- the empirical risk can be used as an impurity measure: the impurity reduction corresponds to the improvement in empirical risk!
- in ID3/C4.5 algorithms: $\mathcal{I} = \widehat{H}$ (information gain)
- in CART: $\mathcal{I} = I_G$

Growing algorithm

```
function GROWTREE($\mathcal{D}$, $l$, $\mathcal{I}$)
    if stopping conditions on $\mathcal{D}$ are fulfilled then
        return the tree $\boxed{\widehat{\mathbf{y}}_l^*(\mathcal{D})}$
    else
        select the best test $f$ according to impurity reduction based on $\mathcal{I}$
        for each possible output of $f$ $o \in \mathcal{O}$ do
            $T_o \leftarrow$ GROWTREE($f(\mathcal{D}, o)$, $l$, $\mathcal{I}$)
        end for
        return the tree
```



```
    end if
end function
```

Selecting the best test

ID3/C4.5

- work only for $|\mathcal{X}_j| < \infty$
- use only $f_n(\mathbf{x}) = x_j$
- the best f is selected by maximizing $\Delta\mathcal{I}(\mathbf{x} \mapsto x_j, \mathcal{D})$ over $j \in \{1, \ldots, P\}$

CART

- more complicated situation
- if $\mathcal{X}_j = \mathbb{R}$
  - sort the values $\{x_j \mid (\mathbf{x}, \mathbf{y}) \in \mathcal{D}\}$ into $(t_i)_{1 \leq i \leq N}$
  - compute all the mid-values, i.e. $\lambda_i = \frac{t_i + t_{i+1}}{2}$
  - select the best f (for $\mathcal{X}_j$) by maximizing $\Delta\mathcal{I}(\mathbf{1}_{x_j \leq \lambda_i}, \mathcal{D})$ over $i \in \{1, \ldots, N-1\}$

Selecting the best test

CART cont.

- if $|\mathcal{X}_j| < \infty$
  - comparing all the tests of the form $\mathbf{1}_{x_j \in A}$ in intractable ($2^{|\mathcal{X}_j|-1} - 1$ possibilities)
  - greedy approach
    - $u^{(1)} = \arg\max_{u \in \mathcal{X}_j} \Delta\mathcal{I}(\mathbf{1}_{x_j = u}, \mathcal{D})$
    - $u^{(2)} = \arg\max_{u \in \mathcal{X}_j \setminus \{u^{(1)}\}} \Delta\mathcal{I}\left(\mathbf{1}_{x_j \in \{u^{(1)}, u\}}, \mathcal{D}\right)$
    - …
    - $u^{(|\mathcal{X}_j|-1)} = \arg\max_{u \in \mathcal{X}_j \setminus \left\{u^{(1)}, \ldots, u^{(|\mathcal{X}_j|-2)}\right\}} \Delta\mathcal{I}\left(\mathbf{1}_{x_j \in \left\{u^{(1)}, \ldots, u^{(|\mathcal{X}_j|-2)}, u\right\}}, \mathcal{D}\right)$
    - select then the best subset from the $\left\{u^{(1)}, \ldots, u^{(k)}\right\}$ over k
  - the greedy approach considers only $\Theta\left(|\mathcal{X}_j|^2\right)$ subsets
  - faster optimal approaches in some particular cases (with $\Theta\left(|\mathcal{X}_j|\right)$ subsets)

Computational complexity

Impurity reduction

- naive approach: $\Theta(|\mathcal{D}|)$ for one test evaluation
- incremental approach: $\Theta(|\mathcal{D}|)$ for a set of tests in some cases

CART

- $\mathcal{X}_j = \mathbb{R}$
  - sorting is in $\Theta(N \log N)$
  - incremental evaluation of the impurity reduction is possible
  - $\Theta(N \log N)$ total
- $|\mathcal{X}_j| < \infty$
  - with $|\mathcal{Y}| = 2$ or $\mathcal{Y} = \mathbb{R}$ (with adapted impurity scores): $\Theta\left(|\mathcal{X}_j|\, N\right)$
  - more costly in arbitrary cases (e.g. $\Theta\left(|\mathcal{X}_j|^2 N^2\right)$
- global: if $|\mathcal{X}_j| \leq N$ and if the tree is balanced $\Theta(N(\log N)^2 P)$

Stopping the growth

Simple stopping conditions

- $|\mathcal{D}| \leq \mathrm{min}_{size}$: do not split small data sets
- if $|\mathcal{Y}| < \infty$, $\mathrm{max}_{\mathbf{y}\in\mathcal{Y}} \widehat{p}(\mathbf{y}, \mathcal{D}) \geq \mathrm{max}_{prob}$: do not split very pure data sets

Advanced stopping conditions

- $\mathrm{min}_{o\in\mathcal{O}} |f(\mathcal{D}, o)| \leq \mathrm{min}_{splitsize}$: do not split when the optimal test produces too small data sets
- $\frac{\Delta\mathcal{I}(f,\mathcal{D})}{\mathcal{I}(\mathcal{D})} \leq \mathrm{min}_{improv}$: do not split when the optimal test does not reduce enough the impurity

Missing data

Missing category

- missing observation for $\mathbf{x}_j \in \mathcal{X}_j$ with $|\mathcal{X}_j| < \infty$
- introduce a new value $\mathcal{X}'_j = \mathcal{X}_j \cap \{NA\}$ that encodes missing data
- proceed normally

Surrogate variables

- exploit local dependency between variables
- once the best test has been found rank all the other tests based on the misclassification error with respect to the output of the test
- store “in the node” a few tests (on distinct variables)
- when a value is missing, use alternative tests

Example

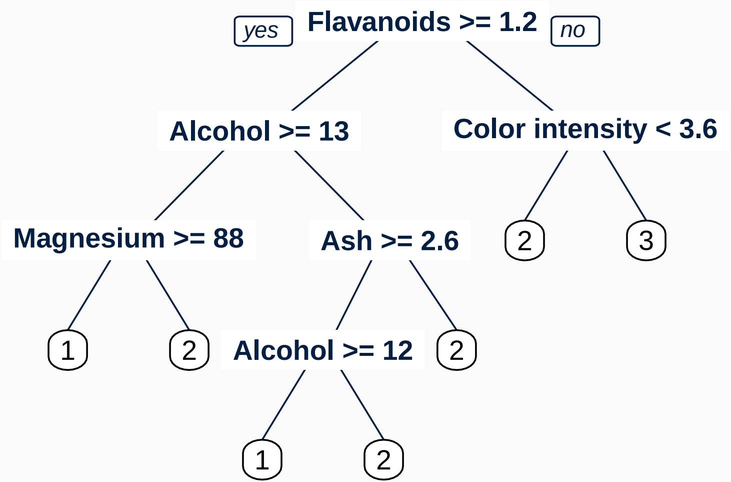
Data: wine

- chemical analysis of wines derived from three cultivars ($\mathcal{Y} = \{1, 2, 3\}$)
- 178 observations with 13 variables ($\mathcal{X} = \mathbb{R}^{13}$)
- $l_b(p, t) = \mathbf{1}_{p \neq t}$
- random split into a $\mathcal{D}$ for learning and $\mathcal{D}'$ for evaluation

Stopping criterion

- $\min_{size} = 2$
- $\min_{improv} = 0$

Example


yes
Flavanoids >= 1.2
no
Alcohol >= 13
Color intensity < 3.6
Magnesium >= 88
Ash >= 2.6
2
3
1
2
Alcohol >= 12
2
1
2

Quality

Confusion matrices

Learning set

	1	2	3
1	30	0	0
2	0	36	0
3	0	0	24

$\widehat{R}_{l_b}(g_T, \mathcal{D})) =$0

Validation set

	1	2	3
1	28	3	4
2	1	32	4
3	0	0	16

$\widehat{R}_{l_b}(g_T, \mathcal{D}') =$0.136

Unbalance

- notice that the data set is unbalanced
- this might explain the relatively poor performances on class 3

Adult data base

Data: Adult

- data extracted from the 1994 US Census
- 13 variables, most of them discrete (i.e. $|\mathcal{X}| < \infty$)
- classification problem: predict whether the annual income of a person is higher or lower than 50K US \$
- 32561 observations in $\mathcal{D}$ for learning
- 16281 observations in $\mathcal{D}'$ for validation/test
- $l_b(p, t) = \mathbf{1}_{p \neq t}$ + weights (re-balancing of the classes)

Results

Parameters

- $\min_{size} = 10$
- $\min_{improv} = 0$

Results

- enormous tree: 1678 leaves
- performances

Learning set

	<=50K	>50K
<=50K	21238	290
>50K	3482	7551

$\widehat{R}_{l_b}(g_T, \mathcal{D})) =$0.116

Validation set

	<=50K	>50K
<=50K	10018	855
>50K	2417	2991

$\widehat{R}_{l_b}(g_T, \mathcal{D}') =$0.201

- some overfitting

Smaller tree

Parameters

- $\min_{size} = 10$
- $\min_{improv} = 0.001$
- smaller tree: 20 leaves

Confusion matrices

Learning set

	<=50K	>50K
<=50K	19747	1161
>50K	4973	6680

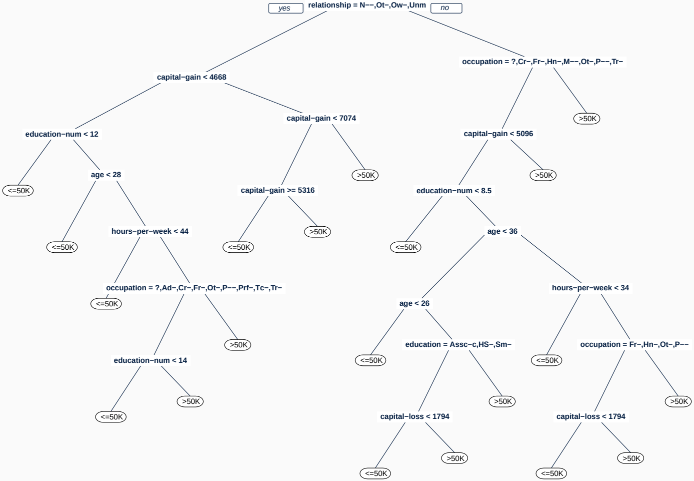
$\widehat{R}_{l_b}(g_T, \mathcal{D}))$ =0.188

Validation set

	<=50K	>50K
<=50K	9955	632
>50K	2480	3214

$\widehat{R}_{l_b}(g_T, \mathcal{D}')$ =0.191

The tree


yes
relationship = N−−,Ot−,Ow−,Unm
no
occupation = ?,Cr−,Fr−,Hn−,M−−,Ot−,P−−,Tr−
capital−gain < 4668
capital−gain < 7074
>50K
education−num < 12
capital−gain < 5096
age < 28
>50K
>50K
<=50K
capital−gain >= 5316
education−num < 8.5
hours−per−week < 44
>50K
age < 36
<=50K
<=50K
<=50K
occupation = ?,Ad−,Cr−,Fr−,Ot−,P−−,Prf−,Tc−,Tr−
hours−per−week < 34
<=50K
age < 26
>50K
education = Assc−c,HS−,Sm−
occupation = Fr−,Hn−,Ot−,P−−
education−num < 14
<=50K
<=50K
>50K
>50K
>50K
<=50K
capital−loss < 1794
capital−loss < 1794
>50K
>50K
<=50K
<=50K

Stopping criteria

From the experiments

- stopping parameters have a strong influence on the performances
- limited knowledge at the decision point:
  - the criteria operate only on a subset of the data
  - at best on a one step ahead basis
- large trees can overfit

Complexity control

- control the size of the tree
- but with a global point of view
- key idea:
  - grow the tree in order to reach a high quality on the training set (possibly with overfitting)
  - then prune the tree using another data set

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Risk vs complexity

Tree complexity

- for a tree T, $|\{\mathbf{y} \in \mathcal{Y} \mid \exists \mathbf{x} \in \mathcal{X}, g_T(\mathbf{x}) = \mathbf{y}\}|$ is finite: it is the number of leaves in T!
- denote $|T|$ this number
- gives a good idea of the complexity of a tree in terms of g_T (rather than in terms of the structure of the tree)

Trade off

- when $|T|$ is large, $\widehat{R}_l(g_T, \mathcal{D})$ is small but the tree is complex and $\widehat{R}_l(g_T, \mathcal{D}')$ might be high
- optimize a compromise between those two aspects

$$C_{l,\alpha}(T, \mathcal{D}) = \widehat{R}_l(g_T, \mathcal{D}) + \alpha |T|$$

Pruning

Two problems

- given α, how to minimize $C_{l,\alpha}(T,\mathcal{D})$ over T in $\mathcal{T}(\mathcal{X},\mathcal{Y})$
- how to chose α

Pruning

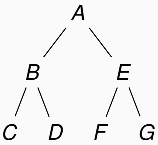
Two problems

- given α, how to minimize $C_{l,\alpha}(T, \mathcal{D})$ over T in $\mathcal{T}(\mathcal{X}, \mathcal{Y})$
- how to chose α

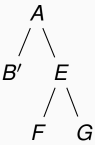
Pruning for $\mathcal{T}(\mathcal{X}, \mathcal{Y})$ exploration

- pruning a tree T consists in replacing any number of its sub-trees by leaves

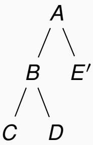
T



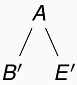
$T' \subset T$



$T'' \subset T$



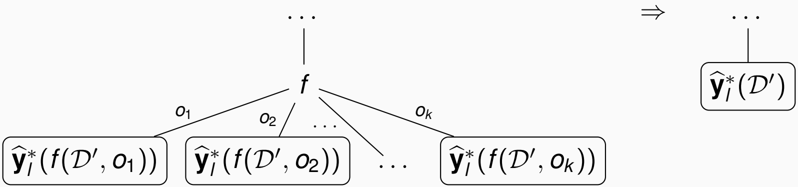
$T''' \subset T'$ and $T''' \subset T''$



Pruning cont.

Pruning decision trees

- best pruning assumption: the value of the leaf that replaces a sub-tree is optimal (risk-wise)
- contextual pruning: a data set is needed to compute the best value $\widehat{\mathbf{y}}_l^*(\mathcal{D})$
- a minimal pruning (when the sub-tree is of height 1) is the exact reverse operation of a growing step of the growing algorithm



$\ldots$
f
o_1
o_2
$\ldots$
o_k
$\widehat{\mathbf{y}}_l^*(f(\mathcal{D}', o_1))$
$\widehat{\mathbf{y}}_l^*(f(\mathcal{D}', o_2))$
$\ldots$
$\widehat{\mathbf{y}}_l^*(f(\mathcal{D}', o_k))$
$\Rightarrow$
$\ldots$
$\widehat{\mathbf{y}}_l^*(\mathcal{D}')$

Optimal tree

Strategy

- from a data set $\mathcal{D}$ grow a complex tree T_{max} (with strict stopping conditions)
- select the optimal tree by solving

$$T^* = \arg \min_{T \subset T_{\text{max}}} C_{l,\alpha}(T, \mathcal{D}) = \arg \min_{T \subset T_{\text{max}}} \left(\widehat{R}_l(g_T, \mathcal{D}) + \alpha \, |T| \right)$$

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Tractable?

- replacing $\mathcal{T}(\mathcal{X}, \mathcal{Y})$ by $\{T \in \mathcal{T}(\mathcal{X}, \mathcal{Y}) \mid T \subset T_{\max}\}$ simplifies tremendously the optimization problem
- but might still be a very large set!

Greedy pruning

Weakest node pruning

- given T consider all the nodes with only leaves as sub-trees
- compute for each such node the modification induced in $C_{l,\alpha}$ by pruning the node
- define $wnp(T)$ as the tree obtained by pruning the node which decreases the most $C_{l,\alpha}$

Greedy (but exact!) algorithm

- $T^{(0)} = T_{\max}$
- $T^{(k)} = wnp\left(T^{(k-1)}\right)$ (until $T^{(k-1)}$ becomes a leaf)
- $T^* = \arg\min_{T\in\left\{T^{(0)},\ldots,T^{(K)}\right\}} C_{l,\alpha}(T,\mathcal{D})$

Remarks

General

- $|T| \leq N$
- if $T' \subset T$, then $|T'| \leq |T| - 1$
- at most N trees to study
- notice than $T' \subset T$ does not imply any ordering between $C_{l,\alpha}(T, \mathcal{D})$ and $C_{l,\alpha}(T', \mathcal{D})$, thus the maximal decrease might actually be an increase

CART

- binary tree only
- pruning a node with only leaves as sub-trees reduces $|T|$ by exactly one
- wnp is determined only by the risk modification
- $\left\{T^{(0)}, \ldots, T^{(K)}\right\}$ does not depend on α

Compared to early stopping...

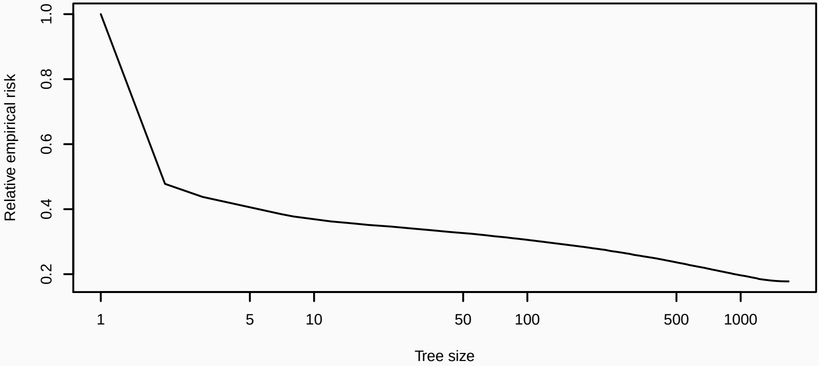
Alternative solution

- use different values of the stopping criterion to produce different trees
- pros and cons:
  - + simpler setting
  - + optimized implementation
  - - opaque parameters: predicting the size of the tree obtained with some parameters is impossible
  - - local decision only
  - - one step ahead only

Example

Adult data set

- $\min_{size} = 10$ and $\min_{improv} = 0$
- 1678 leaves



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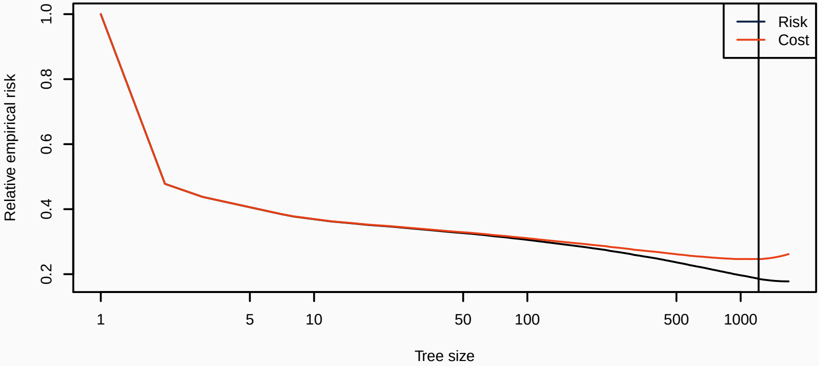

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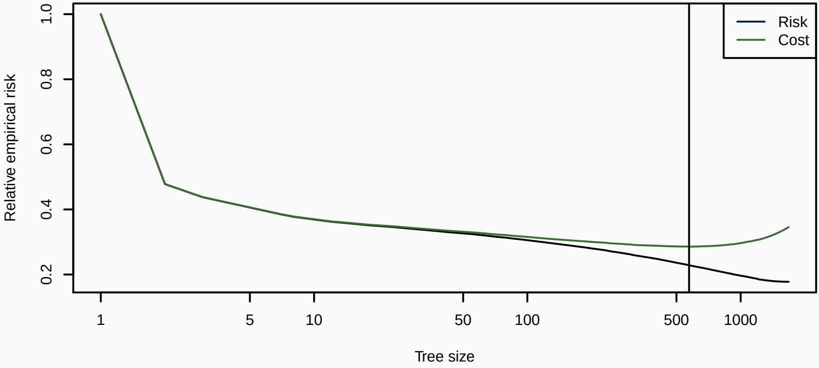

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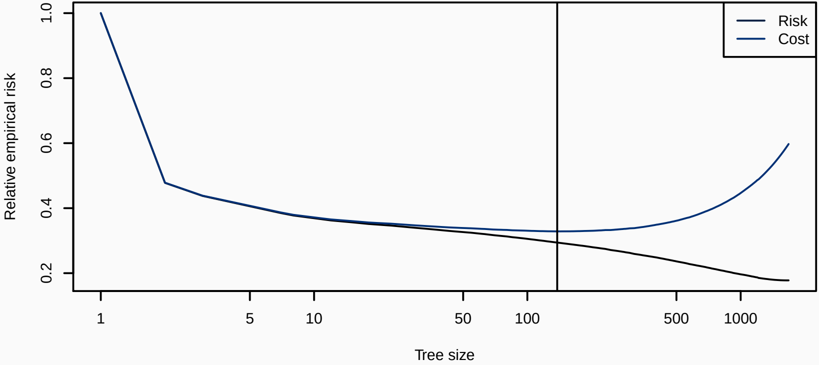

Choosing α

Standard setting!

- the full CART algorithm is given:
  - a data set $\mathcal{D}$
  - a loss function l
  - an impurity measure $\mathcal{I}$
  - α
- and outputs $T^*(\mathcal{D}, l, \mathcal{I}, \alpha)$
- α is a parameter of the algorithm: must be optimized!

Validation approach

- build $T^*(\mathcal{D}, l, \mathcal{I}, \alpha)$ for some αs
- select the best α according to $\widehat{R}_l(g_{T^*(\mathcal{D},l,\mathcal{I},\alpha)}, \mathcal{D}')$

Interresting αs

α sensitivity (case of CART)

- weakest node pruning effect

$$C_{l,\alpha}(T,\mathcal{D}) - C_{l,\alpha}(wnp(T),\mathcal{D}) = \underbrace{\widehat{R}_l(g_T,\mathcal{D}) - \widehat{R}_l(g_{wnp(T)},\mathcal{D})}_{\text{independent of }\alpha} + \alpha$$

- α must be at least equal to $\widehat{R}_l(g_{wnp(T)},\mathcal{D}) - \widehat{R}_l(g_T,\mathcal{D})$ for $wnp(T)$ to be preferred to T
- one can compute intervals such that $T^*(\mathcal{D}, l, \alpha)$ depends only on the interval to which α belongs (cut off values)

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- one can compute intervals such that $T^*(\mathcal{D}, l, \alpha)$ depends only on the interval to which α belongs (cut off values)

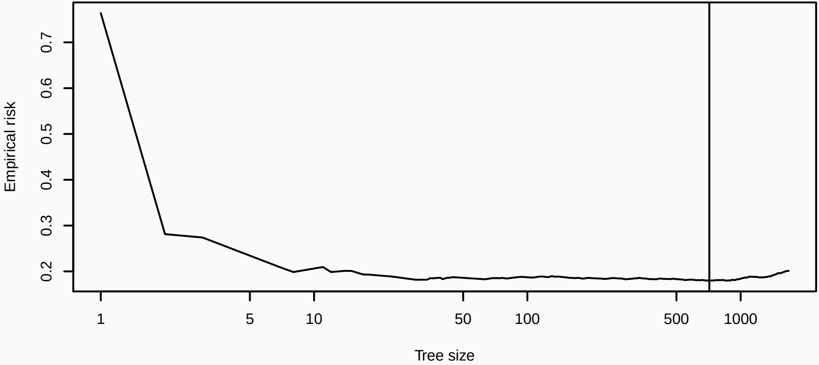
In practice

- in the validation setting, only $\{T^{(0)}, \ldots, T^{(K)}\}$ (does not depend on α)
- in resampling approaches using the intervals is important

Example

Adult data set

- $\mathrm{min}_{size} = 10$ and $\mathrm{min}_{improv} = 0$
- from 1678 leaves to 713



Example

With cross-validation

- 138 leaves
- confusion matrices

Learning set

	<=50K	>50K
<=50K	20164	861
>50K	4556	6980

$\widehat{R}_{l_b}(g_T, \mathcal{D}))$ =0.166

Validation set

	<=50K	>50K
<=50K	9973	612
>50K	2462	3234

$\widehat{R}_{l_b}(g_T, \mathcal{D}')$ =0.189

- full tree

Learning set

	<=50K	>50K
<=50K	21238	290
>50K	3482	7551

$\widehat{R}_{l_b}(g_T, \mathcal{D}))$ =0.116

Validation set

	<=50K	>50K
<=50K	10018	855
>50K	2417	2991

$\widehat{R}_{l_b}(g_T, \mathcal{D}')$ =0.201

Example

With cross-validation

- 138 leaves
- confusion matrices

Learning set

	$<$=50K	$>$50K
$<$=50K	20164	861
$>$50K	4556	6980

$\widehat{R}_{l_b}(g_T, \mathcal{D}))$ =0.166

Validation set

	$<$=50K	$>$50K
$<$=50K	9973	612
$>$50K	2462	3234

$\widehat{R}_{l_b}(g_T, \mathcal{D}')$ =0.189

- small tree (20 leaves)

Learning set

	$<$=50K	$>$50K
$<$=50K	19747	1161
$>$50K	4973	6680

$\widehat{R}_{l_b}(g_T, \mathcal{D}))$ =0.188

Validation set

	$<$=50K	$>$50K
$<$=50K	9955	632
$>$50K	2480	3214

$\widehat{R}_{l_b}(g_T, \mathcal{D}')$ =0.191

CART in summary

```
function CART($\mathcal{D}$, $I$, $\mathcal{I}$)
    $T_{\text{max}} \leftarrow$ GrowTree($\mathcal{D}$, $I$, $\mathcal{I}$)
    $T \leftarrow T_{\text{max}}$
    $Ts \leftarrow \{T_{\text{max}}\}$
    $\alpha s \leftarrow \{\}$
    while $T$ is not a leaf do
        $T \leftarrow wnp(T)$
        $Ts \leftarrow Ts \cup \{T\}$
        compute $\alpha$ the next cut off value
        $\alpha s \leftarrow \alpha s \cup \{\alpha\}$
    end while
    return $(Ts, \alpha s)$
end function
```

And then...

- use a validation technique to select to best tree from *Ts*
- or the best α from αs

Outline

Trees and decision trees

Growing a tree

Pruning a tree

Summary

Decision trees

- simple program like models for machine learning
- pros and cons
  - + relatively fast ($\Theta(N(\log N)^2P)$)
  - + adapted to mixed data
  - + handle missing data
  - + interpretable (for small trees)
  - - medium performances
  - - useful only when interactions between variables are important
  - - highly irregular model (especially for $\mathcal{Y} = \mathbb{R}$)
  - - high variance

Summary

Decision trees

- simple program like models for machine learning
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Combining trees

- trees as building blocks for better algorithms
- bagging, random forests and boosting

Licence

Version

Last git commit: 2018-06-06
By: Fabrice Rossi (Fabrice.Rossi@apiacoa.org)
Git hash: 1b39c1bacfc1b07f96d689db230b2586549a62d4