Boosted decision trees in theory

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Outline

Before we go on...

!!! VERY IMPORTANT !!!

Understand your inputs well
before you start playing with multivariate techniques

Introduction

Decision tree origin

- Machine-learning technique, widely used in social sciences.
  Originally data mining/pattern recognition, then medical diagnostic, insurance/loan screening, etc.

L. Breiman *et al.*, "Classification and Regression Trees" (1984)

Basic principle

- Extend cut-based selection
  - many (most?) events do not have *all* characteristics of signal or background (or we would not be attending SOS2012...)
  - try not to rule out events failing a particular criterion
- Keep events rejected by one criterion and see whether other criteria could help classify them properly

Binary trees

- Trees can be built with branches splitting into many sub-branches
- In this lecture: mostly binary trees

Growing a tree

Tree building algorithm

Start with all events (signal and background) = first (root) node

- sort all events by each variable
- for each variable, find splitting value with best separation between two children
  - mostly signal in one child
  - mostly background in the other
- select variable and splitting value with best separation, produce two branches (nodes)
  - events failing criterion on one side
  - events passing it on the other

Keep splitting

- Now have two new nodes. Repeat algorithm recursively on each node
- Can reuse the same variable
- Iterate until stopping criterion is reached
- Splitting stops: terminal node = leaf

Algorithm example

- Consider signal (s_i) and background (b_j) events described by 3 variables: p_T of leading jet, top mass M_t and scalar sum of p_T's of all objects in the event H_T

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    - $p_T < 56$ GeV, separation $= 3$
    - $H_T < 242$ GeV, separation $= 5$
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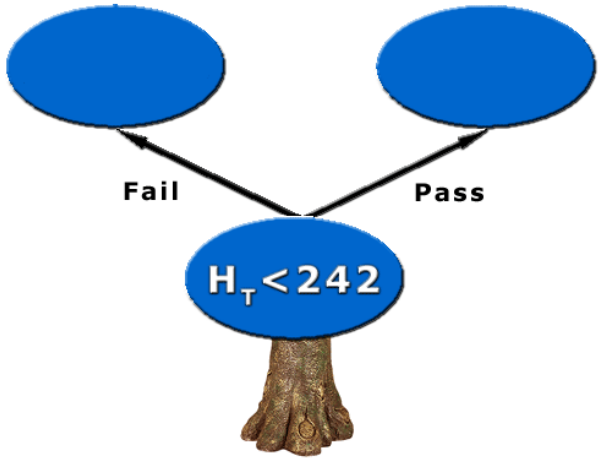

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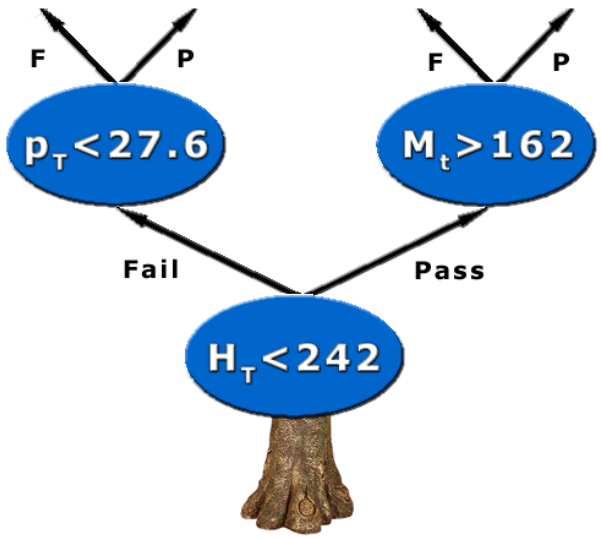

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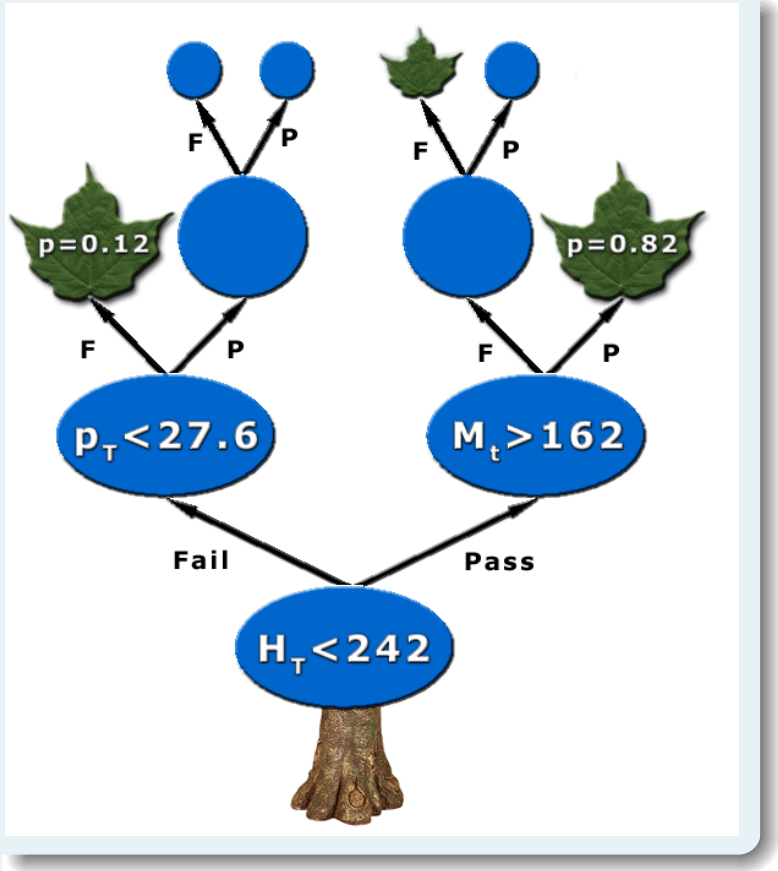


- Repeat recursively on each node
- Splitting stops: e.g. events with $H_T < 242$ GeV and $M_t > 162$ GeV are signal like ($p = 0.82$)

Decision tree output

Run event through tree

- Start from root node
- Apply first best cut
- Go to left or right child node
- Apply best cut for this node
- ...Keep going until...
- Event ends up in leaf

DT Output

- Purity ($\frac{s}{s+b}$, with weighted events) of leaf, close to 1 for signal and 0 for background
- or binary answer (discriminant function $+1$ for signal, -1 or 0 for background) based on purity above/below specified value (e.g. $\frac{1}{2}$) in leaf
- E.g. events with $H_T < 242$ GeV and $M_t > 162$ GeV have a DT output of 0.82 or $+1$

Tree construction parameters

Normalization of signal and background before training

- same total weight for signal and background events ($p = 0.5$, maximal mixing)

Selection of splits

- list of questions ($variable_i < cut_i$?, "Is the sky blue or overcast?")
- goodness of split (separation measure)

Decision to stop splitting (declare a node terminal)

- minimum leaf size (for statistical significance, e.g. 100 events)
- insufficient improvement from further splitting
- perfect classification (all events in leaf belong to same class)
- maximal tree depth (like-size trees choice or computing concerns)

Assignment of terminal node to a class

- signal leaf if purity > 0.5, background otherwise

Splitting a node

Impurity measure i(t)

- maximal for equal mix of signal and background
- symmetric in p_{signal} and $p_{background}$
- minimal for node with either signal only or background only
- strictly concave $\Rightarrow$ reward purer nodes (favours end cuts with one smaller node and one larger node)

Optimal split: figure of merit

- Decrease of impurity for split s of node t into children t_P and t_F (goodness of split):
  $\Delta i(s,t) = i(t) - p_P \cdot i(t_P) - p_F \cdot i(t_F)$
- Aim: find split s^* such that:

$$\Delta i(s^*,t) = \max_{s \in \{\text{splits}\}} \Delta i(s,t)$$

Stopping condition

- See previous slide
- When not enough improvement ($\Delta i(s^*,t) < \beta$)
- Careful with early-stopping conditions

- Maximising $\Delta i(s,t) \equiv$ minimizing overall tree impurity

Splitting a node: examples

Node purity

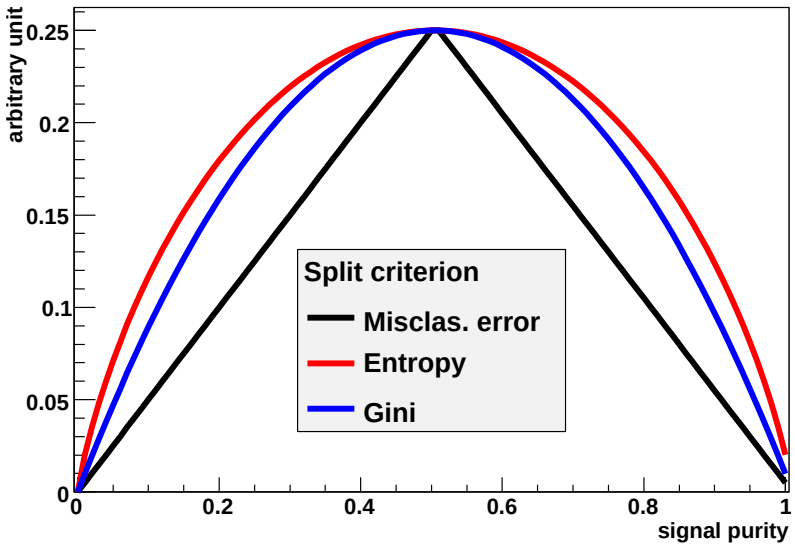
- Signal (background) event i with weight w_s^i (w_b^i)

$$p = \frac{\sum_{i \in signal} w_s^i}{\sum_{i \in signal} w_s^i + \sum_{j \in bkg} w_b^j}$$

- Signal purity (= purity)
  $p_s = p = \frac{s}{s+b}$
- Background purity
  $p_b = \frac{b}{s+b} = 1 - p_s = 1 - p$

Common impurity functions

- misclassification error
  $= 1 - max(p, 1-p)$
- (cross) entropy
  $= -\sum_{i=s,b} p_i \log p_i$
- Gini index



- Also cross section ($-\frac{s^2}{s+b}$) and excess significance ($-\frac{s^2}{b}$)

Splitting a node: Gini index of diversity

Defined for many classes

- Gini $= \sum_{i,j\in\{\text{classes}\}}^{i\neq j} p_i p_j$

Statistical interpretation

- Assign random object to class i with probability p_i.
- Probability that it is actually in class j is p_j
- $\Rightarrow$ Gini = probability of misclassification

For two classes (signal and background)

- $i = s, b$ and $p_s = p = 1 - p_b$
- $\Rightarrow$ Gini $= 1 - \sum_{i=s,b} p_i^2 = 2p(1-p) = \frac{2sb}{(s+b)^2}$
- Most popular in DT implementations
- Usually similar performance to e.g. entropy

Variable selection I

Reminder

- Need model giving good description of data

Variable selection I

Reminder

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Playing with variables

- Number of variables:
  - not affected too much by "curse of dimensionality"
  - CPU consumption scales as $nN \log N$ with n variables and N training events
- Insensitive to duplicate variables (give same ordering $\Rightarrow$ same DT)
- Variable order does not matter: all variables treated equal
- Order of training events is irrelevant
- Irrelevant variables:
  - no discriminative power (e.g. age of analyst) $\Rightarrow$ not used
  - only costs a little CPU time, no added noise
- Can use continuous and discrete variables, simultaneously

Variable selection II

Transforming input variables

- Completely insensitive to the replacement of any subset of input variables by (possibly different) arbitrary strictly monotone functions of them:
  - let $f : x_i \rightarrow f(x_i)$ be strictly monotone
  - if $x > y$ then $f(x) > f(y)$
  - ordering of events by x_i is the same as by $f(x_i)$
  - $\Rightarrow$ produces the same DT
- Examples:
  - convert MeV $\rightarrow$ GeV
  - no need to make all variables fit in the same range
  - no need to regularise variables (e.g. taking the log)
- $\Rightarrow$ Some immunity against outliers

Variable selection III

Linear combinations of input variables

- Until now, answering questions like "is $x_i < c_i$?"
- Instead, take set of coefficients $a = (a_1, .., a_n)$, $||a||^2 = \sum_i a_i^2 = 1$
- Question: "is $\sum_i a_i x_i < c_i$?"
- Choose optimal split $s^*(a^*)$ and set of linear coefficients a^* that maximises $\Delta i(s^*(a), t)$
- Tricky to implement, very CPU intensive
- Only useful with *strong linear correlations* $\Rightarrow$ better to decorrelate first. DT will find them anyway, but inefficiently. (Be careful with decorrelation if non-linear)

Variable ranking

- Ranking of variable x_i: add up decrease of impurity at each node where x_i is used
- Largest decrease of impurity = best variable

Variable selection IV

Shortcoming: masking of variables

- x_j may be just a little worse than x_i but will never be picked
- x_j is ranked as irrelevant
- But remove x_i and x_j becomes very relevant
  $\Rightarrow$ careful with interpreting ranking

Solution: surrogate split

- Compare which events are sent left or right by optimal split and by any other split
- Give higher score to split that mimics better the optimal split
- Highest score = surrogate split
- Can be included in variable ranking
- Helps in case of missing data: replace optimal split by surrogate

Tree (in)stability

Tree instability

Training sample composition

- Small changes in sample can lead to very different tree structures
- Performance on testing events may be as good, or not
- Not optimal to understand data from DT rules
- Doesn't give confidence in result:
  - DT output distribution discrete by nature
  - granularity related to tree complexity
  - tendency to have spikes at certain purity values (or just two delta functions at ± 1 if not using purity)

Pruning a tree I

Why prune a tree?

- Possible to get a perfect classifier on training events
- Mathematically misclassification error can be made as little as wanted
- E.g. tree with one class only per leaf (down to 1 event per leaf if necessary)
- Training error is zero
- But run new independent events through tree (testing or validation sample): misclassification is probably > 0, overtraining
- Pruning: eliminate subtrees (branches) that seem too specific to training sample:
  - a node and all its descendants turn into a leaf

Pruning a tree II

Pre-pruning

- Stop tree growth during building phase
- Already seen: minimum leaf size, minimum separation improvement, maximum depth, etc.
- Careful: early stopping condition may prevent from discovering further useful splitting

Expected error pruning

- Grow full tree
- When result from children not significantly different from result of parent, prune children
- Can measure statistical error estimate with binomial error $\sqrt{p(1-p)/N}$ for node with purity p and N training events
- No need for testing sample
- Known to be "too aggressive"

Pruning a tree III

Cost-complexity pruning

- Idea: penalise "complex" trees (many nodes/leaves) and find compromise between good fit to training data (larger tree) and good generalisation properties (smaller tree)
- With misclassification rate $R(T)$ of subtree T (with N_T nodes) of fully grown tree T_{max}:

$$\text{cost complexity } R_\alpha(T) = R(T) + \alpha N_T$$

  $\alpha =$ complexity parameter
- Minimise $R_\alpha(T)$:
  - small α: pick T_{max}
  - large α: keep root node only, T_{max} fully pruned
- First-pass pruning, for terminal nodes t_L, t_R from split of t:
  - by construction $R(t) \geq R(t_L) + R(t_R)$
  - if $R(t) = R(t_L) + R(t_R)$ prune off t_L and t_R

Pruning a tree IV

Cost-complexity pruning

- For node t and subtree T_t:
  - if t non-terminal, $R(t) > R(T_t)$ by construction
  - $R_\alpha(\{t\}) = R_\alpha(t) = R(t) + \alpha$ ($N_T = 1$)
  - if $R_\alpha(T_t) < R_\alpha(t)$ then branch has smaller cost-complexity than single node and should be kept
  - at critical $\alpha = \rho_t$, node is preferable
  - to find ρ_t, solve $R_{\rho_t}(T_t) = R_{\rho_t}(t)$, or: $\rho_t = \dfrac{R(t) - R(T_t)}{N_T - 1}$
  - node with smallest ρ_t is *weakest link* and gets pruned
  - apply recursively till you get to the root node
- This generates sequence of decreasing cost-complexity subtrees
- Compute their true misclassification rate on validation sample:
  - will first decrease with cost-complexity
  - then goes through a minimum and increases again
  - pick this tree at the minimum as the best pruned tree

- Note: best pruned tree may not be optimal in a forest

Decision tree score card

✔ Training is fast

✔ Human readable (not a black box, can interpret tree as selection rules or physics)

✔ Deals with continuous and discrete variables simultaneously

✔ No need to transform inputs

✔ Resistant to irrelevant variables

✔ Works well with many variables

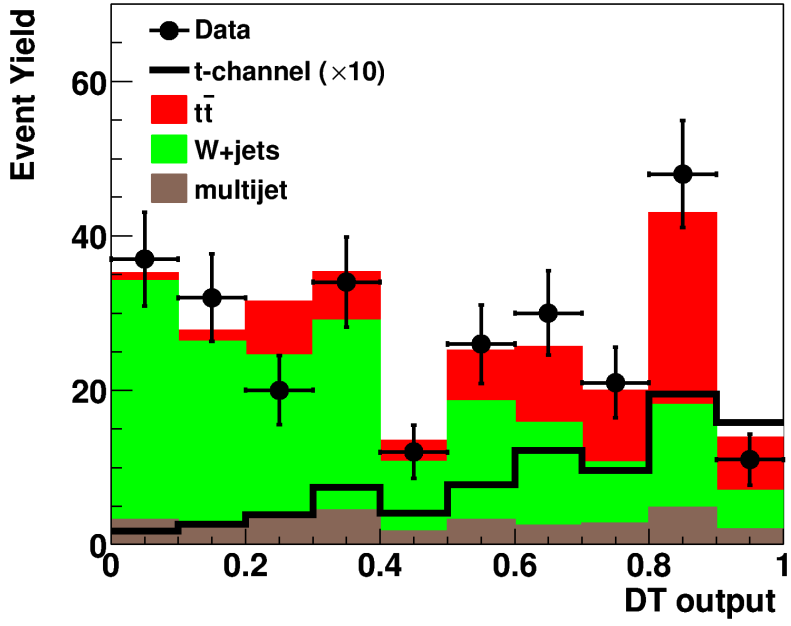
✘✔ Good variables can be masked

✔ Very few parameters

✔✘ Less and less "original" in HEP

✘ Unstable tree structure

✘ Piecewise nature of output



Tree (in)stability solution

Averaging

- Build several trees and average the output
- V-fold cross-validation (good for small samples)
  - divide training sample $\mathcal{L}$ in V subsets of equal size: $\mathcal{L} = \bigcup_{v=1..V} \mathcal{L}_v$
  - Train tree T_v on $\mathcal{L} - \mathcal{L}_v$, test on $\mathcal{L}_v$
  - DT output $= \frac{1}{V} \sum_{v=1..V} T_v$
- Bagging, boosting, random forests, etc.

Boosting

A brief history of boosting

First provable algorithm by Schapire (1990)

- Train classifier T_1 on N events
- Train T_2 on new N-sample, half of which misclassified by T_1
- Build T_3 on events where T_1 and T_2 disagree
- Boosted classifier: MajorityVote(T_1, T_2, T_3)

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- Freund&Schapire joined forces: 1st functional model AdaBoost (1996)

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"Recently" in HEP

- MiniBooNe compared performance of different boosting algorithms and neural networks for particle ID (2005)
- D0 claimed first evidence for single top quark production (2006)
- CDF copied (2008). Both used BDT for single top observation

Principles of boosting

What is boosting?

- General method, not limited to decision trees
- Hard to make a very good learner, but easy to make simple, error-prone ones (but still better than random guessing)
- Goal: combine such weak classifiers into a new more stable one, with smaller error

Algorithm

- Training sample $\mathbb{T}_k$ of N events. For i^{th} event:
  - weight w_i^k
  - vector of discriminative variables x_i
  - class label $y_i = +1$ for signal, -1 for background
- Pseudocode:

  Initialise $\mathbb{T}_1$
  for k in $1..N_{tree}$
    train classifier T_k on $\mathbb{T}_k$
    assign weight α_k to T_k
    modify $\mathbb{T}_k$ into $\mathbb{T}_{k+1}$
- Boosted output: $F(T_1, .., T_{N_{tree}})$

AdaBoost

What is AdaBoost?

- Introduced by Freund&Schapire in 1996
- Stands for *adaptive boosting*
- Learning procedure adjusts to training data to classify it better
- Many variations on the same theme for actual implementation
- Most common boosting algorithm around
- Usually leads to better results than without boosting

AdaBoost algorithm

- Check which events of training sample $\mathbb{T}_k$ are misclassified by T_k:
  - $\mathbb{I}(X) = 1$ if X is true, 0 otherwise
  - for DT output in $\{\pm 1\}$: $\text{isMisclassified}_k(i) = \mathbb{I}\big(y_i \times T_k(x_i) \leq 0\big)$
  - or $\text{isMisclassified}_k(i) = \mathbb{I}\big(y_i \times (T_k(x_i) - 0.5) \leq 0\big)$ in purity convention
  - misclassification rate:

$$R(T_k) = \epsilon_k = \frac{\sum_{i=1}^{N} w_i^k \times \text{isMisclassified}_k(i)}{\sum_{i=1}^{N} w_i^k}$$

- Derive tree weight $\alpha_k = \beta \times \ln((1-\epsilon_k)/\epsilon_k)$
- Increase weight of misclassified events in $\mathbb{T}_k$ to create $\mathbb{T}_{k+1}$:

$$w_i^k \rightarrow w_i^{k+1} = w_i^k \times e^{\alpha_k}$$

- Train T_{k+1} on $\mathbb{T}_{k+1}$
- Boosted result of event i:

$$T(i) = \frac{1}{\sum_{k=1}^{N_{\text{tree}}} \alpha_k} \sum_{k=1}^{N_{\text{tree}}} \alpha_k T_k(i)$$

AdaBoost by example

- Assume $\beta = 1$

Not-so-good classifier

- Assume error rate $\epsilon = 40\%$
- Then $\alpha = \ln \frac{1-0.4}{0.4} = 0.4$
- Misclassified events get their weight multiplied by $e^{0.4}$=1.5
- $\Rightarrow$ next tree will have to work a bit harder on these events

Good classifier

- Error rate $\epsilon = 5\%$
- Then $\alpha = \ln \frac{1-0.05}{0.05} = 2.9$
- Misclassified events get their weight multiplied by $e^{2.9}$=19 (!!)
- $\Rightarrow$ being failed by a good classifier means a big penalty:
  - must be a difficult case
  - next tree will have to pay much more attention to this event and try to get it right

AdaBoost error rate

Misclassification rate ϵ on training sample

- Can be shown to be bound:
$$\epsilon \leq \prod_{k=1}^{N_{tree}} 2\sqrt{\epsilon_k(1-\epsilon_k)}$$
- If each tree has $\epsilon_k \neq 0.5$ (i.e. better than random guessing):

  the error rate falls to zero for sufficiently large N_{tree}

- Corollary: training data is over fitted

Overtraining? (more tomorrow)

- Error rate on test sample may reach a minimum and then potentially rise. Stop boosting at the minimum.
- In principle AdaBoost *must* overfit training sample
- In many cases in literature, no loss of performance due to overtraining
  - may have to do with fact that successive trees get in general smaller and smaller weights
  - trees that lead to overtraining contribute very little to final DT output on validation sample

Other boosting algorithms

ϵ-Boost (shrinkage)

- reweight misclassified events by a fixed $e^{2\epsilon}$ factor
- $T(i) = \sum_{k=1}^{N_{\text{tree}}} \epsilon T_k(i)$

ϵ-LogitBoost

- reweight misclassified events by logistic function $\frac{e^{-y_i T_k(x_i)}}{1+e^{-y_i T_k(x_i)}}$
- $T(i) = \sum_{k=1}^{N_{\text{tree}}} \epsilon T_k(i)$

Real AdaBoost

- DT output is $T_k(i) = 0.5 \times \ln \frac{p_k(i)}{1-p_k(i)}$ where $p_k(i)$ is purity of leaf on which event i falls
- reweight events by $e^{-y_i T_k(i)}$
- $T(i) = \sum_{k=1}^{N_{\text{tree}}} T_k(i)$

- ϵ-HingeBoost, LogitBoost, Gentle AdaBoost, etc.

Other averaging techniques

Bagging (Bootstrap aggregating)

- Before building tree T_k take random sample of N events from training sample with replacement
- Train T_k on it
- Events not picked form "out of bag" validation sample

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- Two levels of randomisation, much more stable output

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Trimming

- Not exactly the same. Used to speed up training
- After some boosting, very few high weight events may contribute
- $\Rightarrow$ ignore events with too small a weight

Conclusion

- Decision trees have been around for some time in social sciences
- Natural extension to cut-based analysis
- Greatly improved performance with boosting (and also with bagging, random forests)
- Becoming rather fashionable in HEP
- Even so, expect a lot of scepticism: you'll have to convince people that your advanced technique leads to meaningful and reliable results $\Rightarrow$ ensemble tests, use several techniques, compare to random grid search, etc.
- As with other advanced techniques, no point in using them if data are not understood and well modelled
- Even less point optimising MVA to death if you have no data...

References I


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