Boosted decision trees

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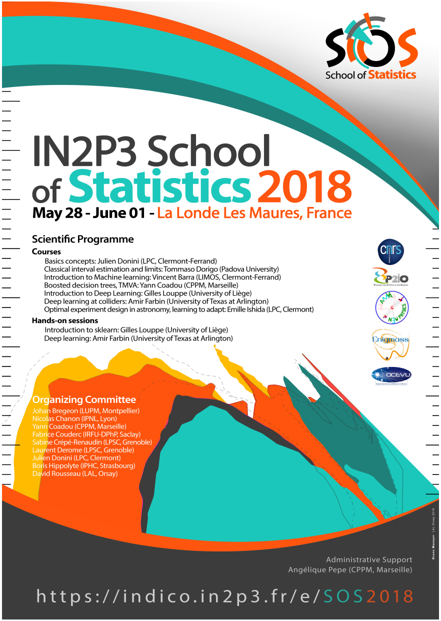
Outline



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Before we go on...

!!! VERY IMPORTANT !!!

Understand your inputs well
before you start playing with
multivariate techniques and machine learning

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
  - 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

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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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    - $p_T^{s_1} \leq p_T^{b_{34}} \leq \cdots \leq p_T^{b_2} \leq p_T^{s_{12}}$
    - $H_T^{b_5} \leq H_T^{b_3} \leq \cdots \leq H_T^{s_{67}} \leq H_T^{s_{43}}$
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  - best split (arbitrary unit):
    - $p_T < 56$ GeV, separation $= 3$
    - $H_T < 242$ GeV, separation $= 5$
    - $M_t < 105$ GeV, separation $= 0.7$

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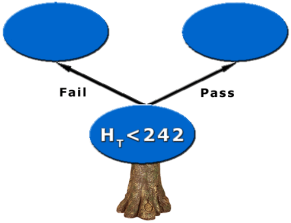

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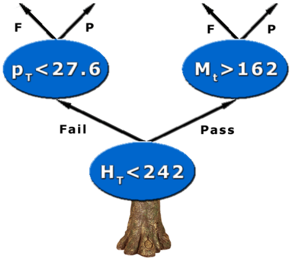
- Repeat recursively on each node



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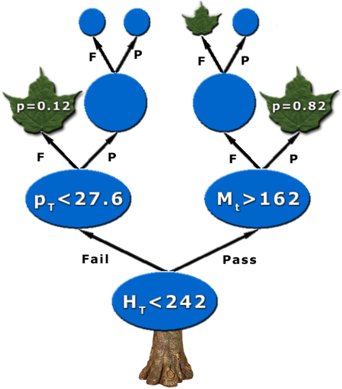
- Splitting stops: e.g. events with $H_T < 242$ GeV and $M_t > 162$ GeV are signal like ($p = 0.82$)



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 $\left(\frac{s}{s+b}\right.$, with weighted events$\left.\right)$ 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

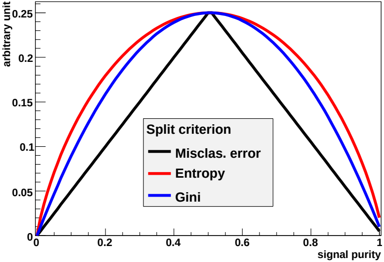
- Signal (background) event i with weight w_s^i (w_b^i)

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

- 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 (details in backup)



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

Variable selection I

Reminder

- Need model giving good description of data

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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 (batch training)
- Irrelevant variables:
  - no discriminative power $\Rightarrow$ 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 $f : x_i \to f(x_i)$ 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 $\to$ 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

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Note about actual implementation

- The above is strictly true only if testing all possible cut values
- If there is some computational optimisation (e.g., check only 20 possible cuts on each variable), it may not work anymore

Variable selection III

Variable ranking

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

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

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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
- Does not 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

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 algorithms (details in backup)

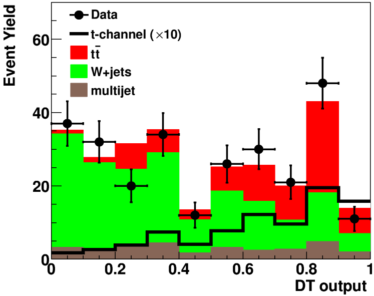
- Pre-pruning (early stopping condition like min leaf size, max depth)
- Expected error pruning (based on statistical error estimate)
- Cost-complexity pruning (penalise “complex” trees with many nodes/leaves)

Decision tree score card

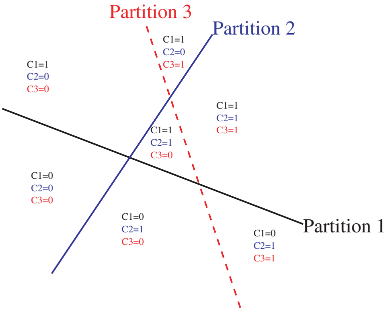
- ✔ Training is fast
- ✔ Human readable (not a black box, can interpret tree as selection rules or physics)

- ✔ 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
- ✔✘ Not that "original" in HEP anymore
- ✘ Unstable tree structure
- ✘ Piecewise nature of output
- ✘ Need at least as many training examples as variations in target function

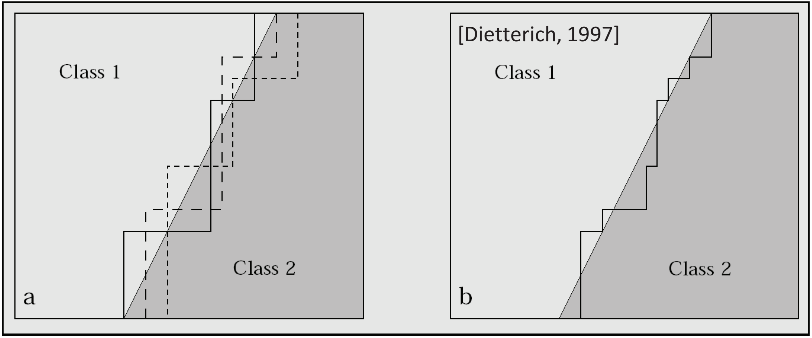


- One tree:
  - one information about event (one leaf)
  - cannot really generalise to variations not covered in training set (at most as many leaves as input size)
- Many trees:
  - distributed representation: number of intersections of leaves exponential in number of trees
  - many leaves contain the event ⇒ richer description of input pattern



Tree (in)stability solution: averaging

- Build several trees and average the output



- K-fold cross-validation (good for small samples)
  - divide training sample $\mathcal{L}$ in K subsets of equal size: $\mathcal{L} = \bigcup_{k=1..K} \mathcal{L}_k$
  - Train tree T_k on $\mathcal{L} - \mathcal{L}_k$, test on $\mathcal{L}_k$
  - DT output $= \frac{1}{K} \sum_{k=1..K} T_k$
- Bagging, boosting, random forests, etc.

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Boosting: a brief history

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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When it really picked up 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

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

- 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:

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

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

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

- 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 $\varepsilon = 40\%$
- 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 $\varepsilon = 5\%$
- 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:
$$\varepsilon \leq \prod_{k=1}^{N_{tree}} 2\sqrt{\varepsilon_k(1-\varepsilon_k)}$$
- If each tree has $\varepsilon_k \neq 0.5$ (i.e. better than random guessing):

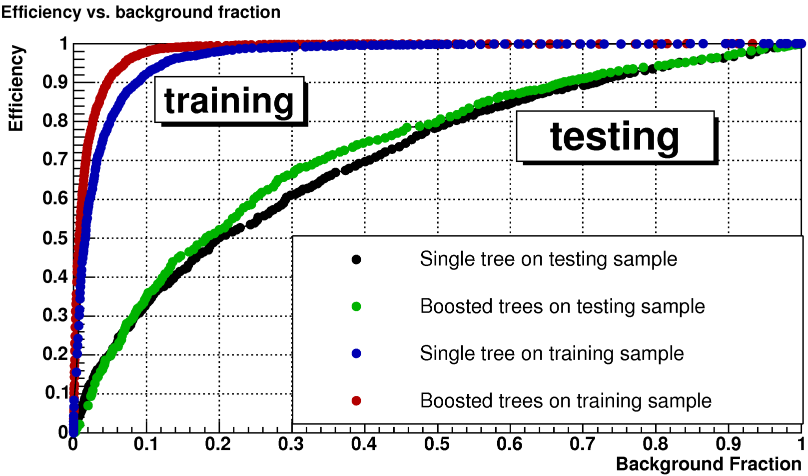
the error rate falls to zero for sufficiently large N_{tree}

- Corollary: training data is over fitted

Overtraining?

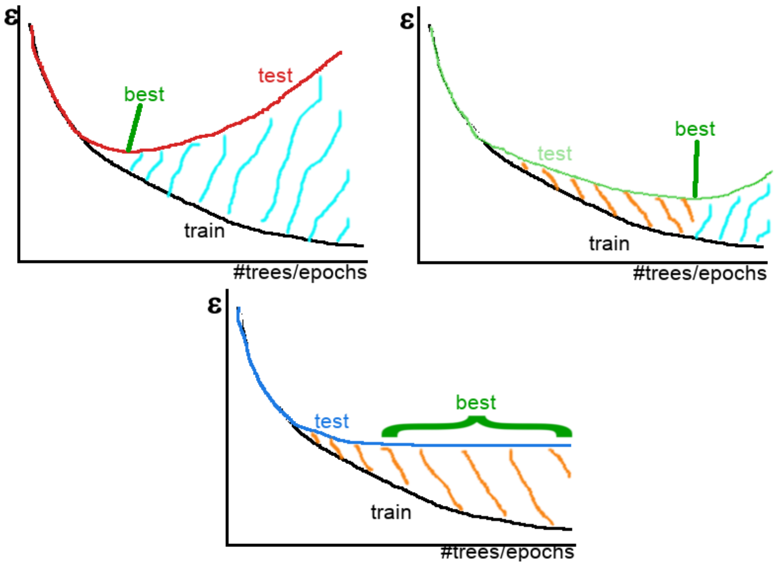
- Error rate on test sample may reach a minimum and then potentially rise. Stop boosting at the minimum.
- In principle AdaBoost *must* overfit training sample
- In many cases in literature, no loss of performance due to overtraining
  - may have to do with fact that successive trees get in general smaller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

Training and generalisation error



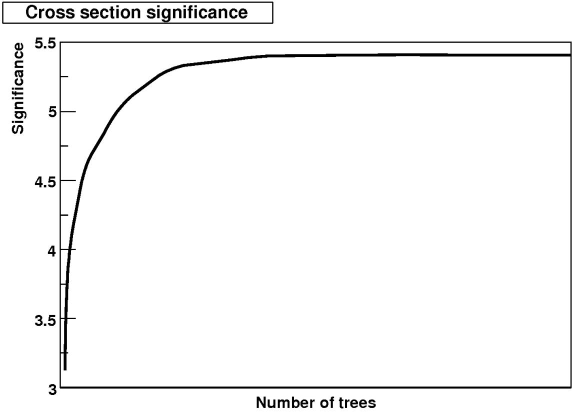
- Clear overtraining, but still better performance after boosting

Overtraining estimation: good or bad?



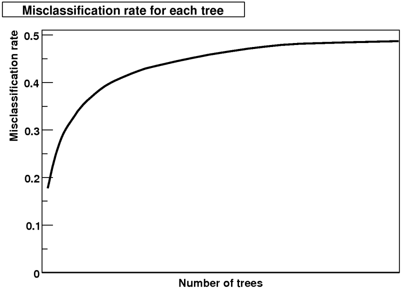
"good" overtraining / "bad" overtraining

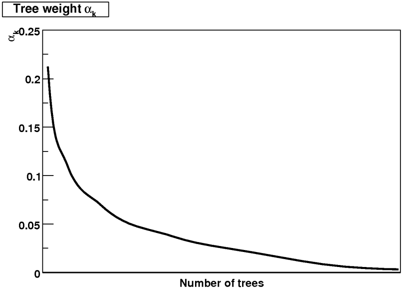
Cross section significance $(s/\sqrt{s+b})$



- More relevant than testing error
- Reaches plateau
- Afterwards, boosting does not hurt (just wasted CPU)
- Applicable to any other figure of merit of interest for your use case

Clues to boosting performance





- First tree is best, others are minor corrections
- Specialised trees do not perform well on most events $\Rightarrow$ decreasing tree weight and increasing misclassification rate
- Last tree is not better evolution of first tree, but rather a pretty bad DT that only does a good job on few cases that the other trees could not get right

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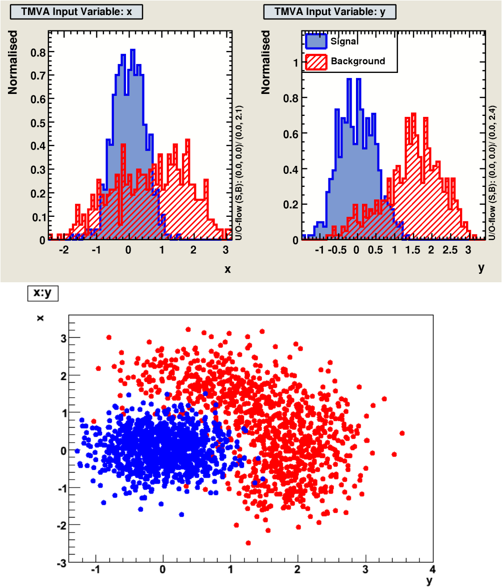
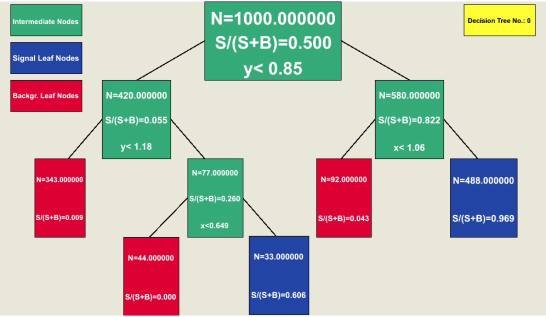
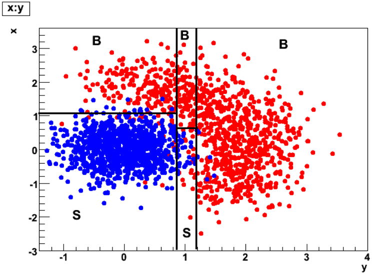
Concrete example

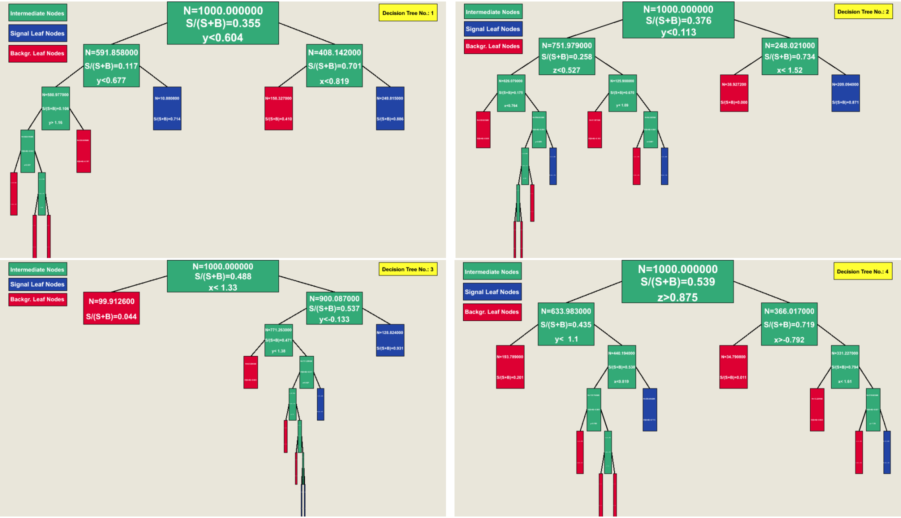


Concrete example



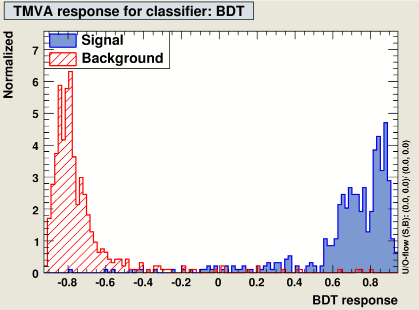


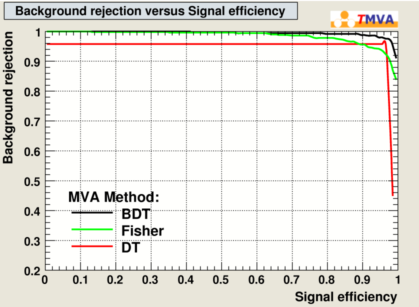
Concrete example



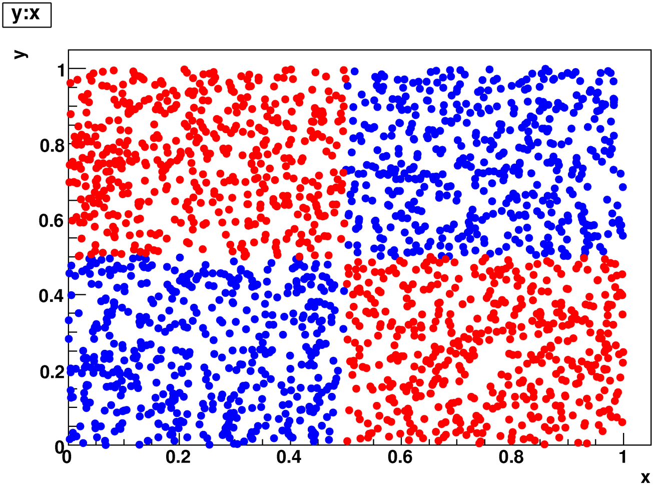
- Specialised trees

Concrete example

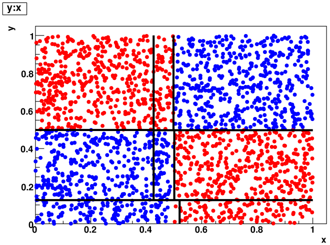


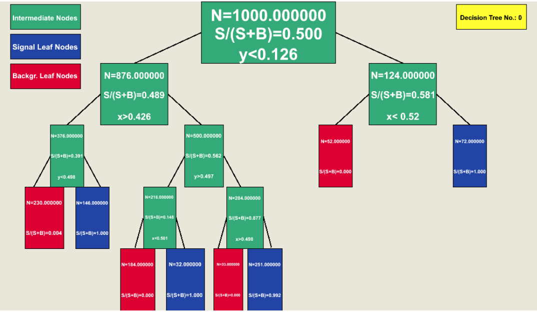


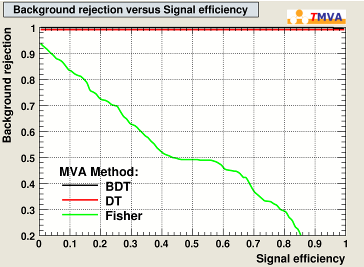
Concrete example: XOR



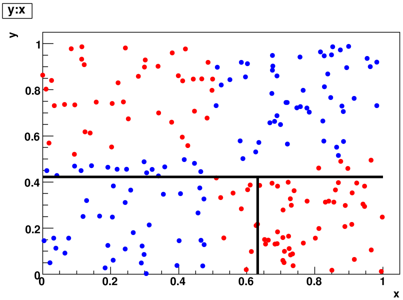
Concrete example: XOR





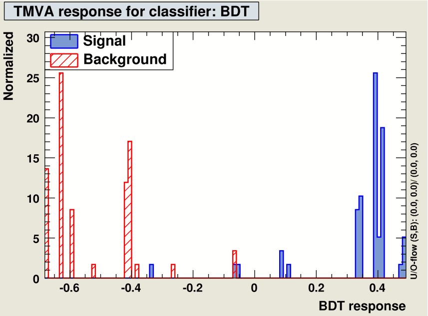


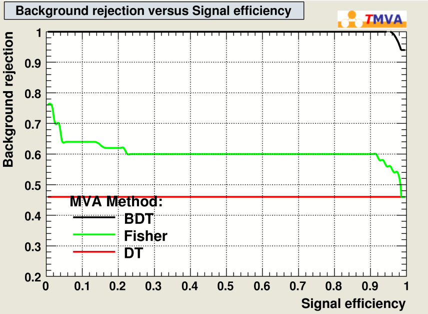
Concrete example: XOR with 100 events



Small statistics

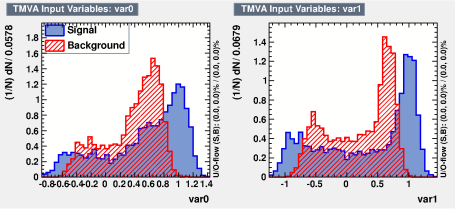
- Single tree or Fischer discriminant not so good
- BDT very good: high performance discriminant from combination of weak classifiers

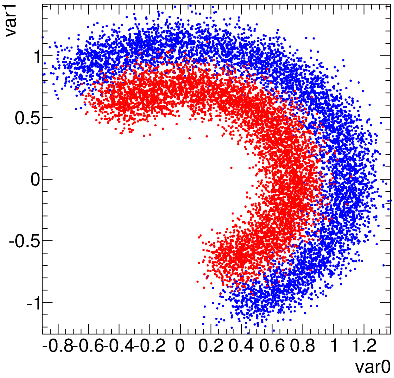




Circular correlation

- Using TMVA and `create_circ` macro from `$ROOTSYS/tutorials/tmva/createData.C` to generate dataset
- Plots: `TMVA::TMVAGui("filename")`

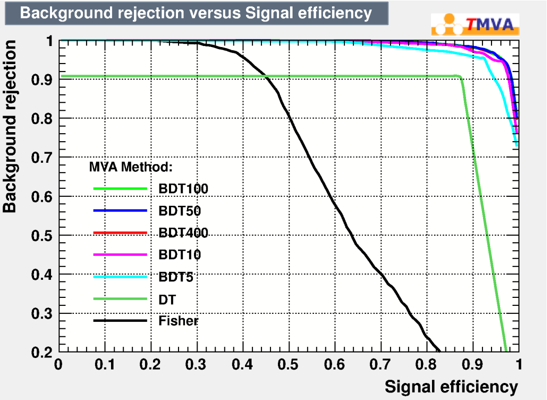




Circular correlation

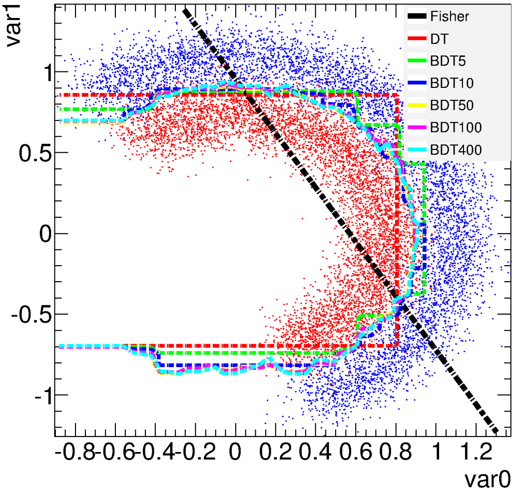
Boosting longer (TMVA: `NTrees`)

- Compare performance of Fisher discriminant, single DT and BDT with more and more trees (5 to 400)
- All other parameters at TMVA default (would be 400 trees)



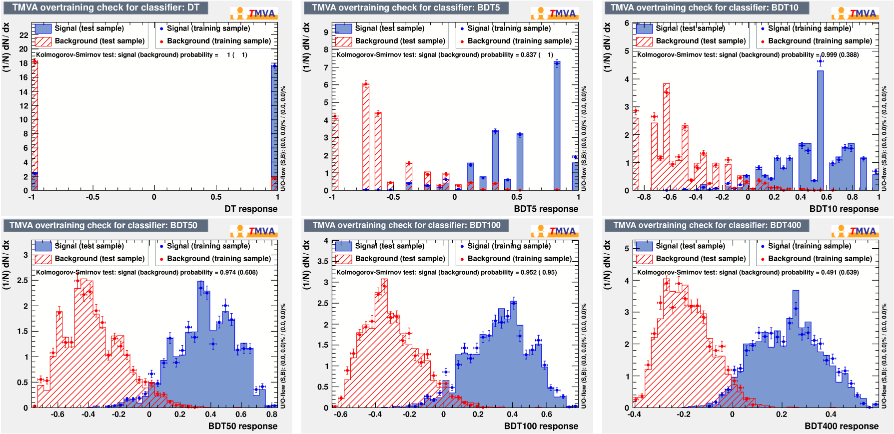
- Fisher bad (expected)
- Single (small) DT: not so good
- More trees ⇒ improve performance until saturation

Decision contours



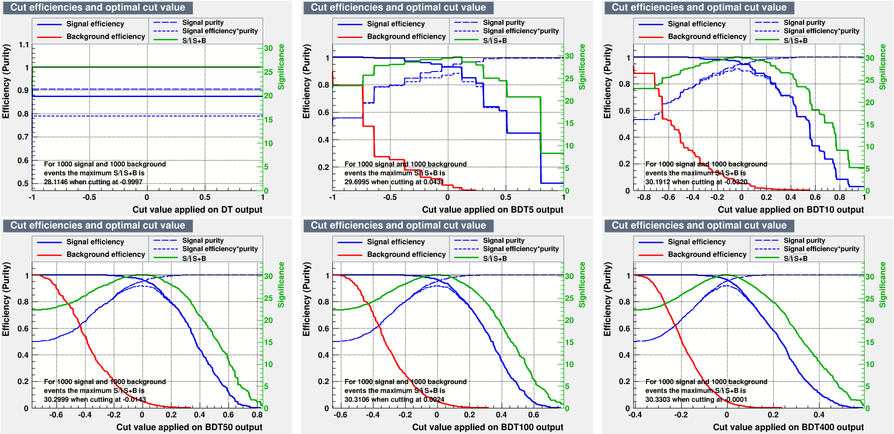
- Fisher bad (expected)
- Note: max tree depth = 3
- Single (small) DT: not so good. Note: a larger tree would solve this problem
- More trees ⇒ improve performance (less step-like, closer to optimal separation) until saturation
- Largest BDTs: wiggle a little around the contour ⇒ picked up features of training sample, that is, overtraining

Training/testing output



- Better shape with more trees: quasi-continuous
- Overtraining because of disagreement between training and testing? Let's see

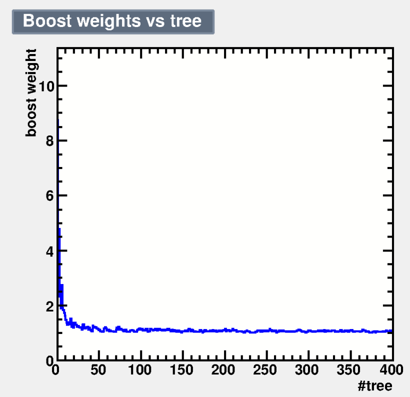
Performance in optimal significance

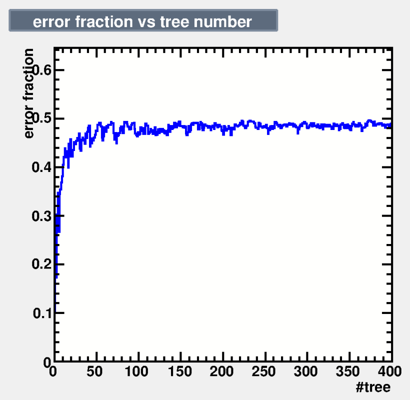


- Best significance actually obtained with last BDT, 400 trees!
- But to be fair, equivalent performance with 10 trees already
- Less “stepped” output desirable? $\Rightarrow$ maybe 50 is reasonable

Control plots

- Boosting weight decreases fast and stabilises
- First trees have small error fractions, then increases towards 0.5 (random guess)
- ⇒ confirms that best trees are first ones, others are small corrections

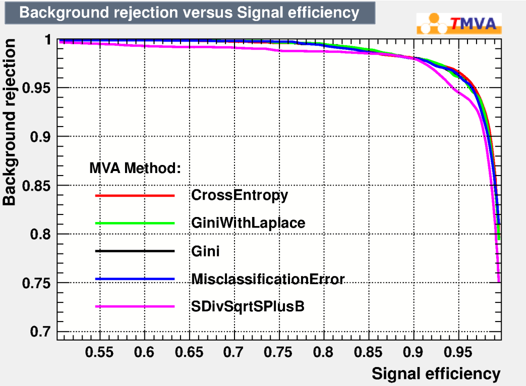




Circular correlation

Separation criterion for node splitting (TMVA: `SeparationType`)

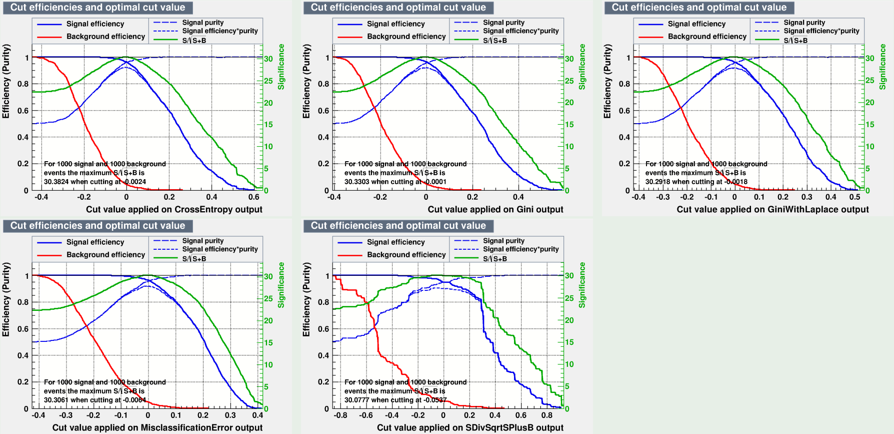
- Compare performance of Gini, entropy, misclassification error, $\frac{s}{\sqrt{s+b}}$
- All other parameters at TMVA default



- Very similar performance (even zooming on corner)
- Small degradation (in this particular case) for $\frac{s}{\sqrt{s+b}}$: only criterion that does not respect good properties of impurity measure (see earlier: maximal for equal mix of signal and bkg, symmetric in p_{sig} and p_{bkg}, minimal for node with either signal only or bkg only, strictly concave)

Circular correlation

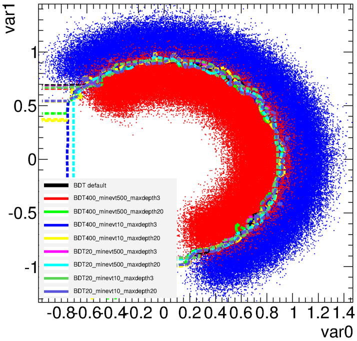
Performance in optimal significance

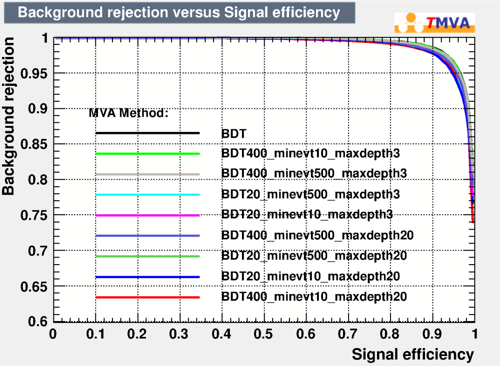


- Confirms previous page: very similar performance, worse for BDT optimised with significance!

Many small trees or fewer large trees?

- Using same `create_circ` macro but generating larger dataset to avoid stats limitations
- 20 or 400 trees; minimum leaf size: 10 or 500 events (`MinNodeSize`)
- Maximum depth (max # of cuts to reach leaf): 3 or 20 (`MaxDepth`)





- Overall: very comparable performance. Depends on use case.

- **TMVA**: Toolkit for MultiVariate Analysis
- http://tmva.sourceforge.net https://github.com/root-project/root/tree/master/tmva
- Written by physicists
- In C++ (also python API), integrated in ROOT
- Quite complete manual
- Includes many different multivariate/machine learning techniques
- To compile, add appropriate header files in your code (e.g., `#include "TMVA/Factory.h"`) and this to your compiler command line: `` `root-config --cflags --libs --glibs` -lTMVA ``
- More complete examples of code: `$ROOTSYS/tutorials/tmva`
  - `createData.C` macro to make example datasets
  - classification and regression macros
  - also includes Keras examples (deep learning)
- Sometimes useful performance measures (more in these headers):

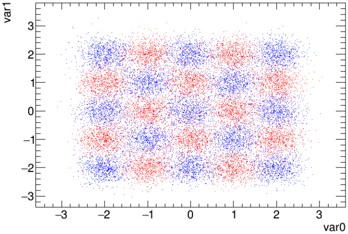
```
#include "TMVA/ROCCalc.h"
TMVA::ROCCalc(TH1* S,TH1* B).GetROCIntegral();
#include "TMVA/Tools.h"
TMVA::gTools().GetSeparation(TH1* S,TH1* B);
```

Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
```

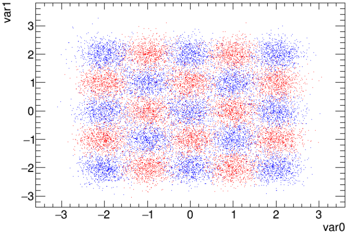
Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
```



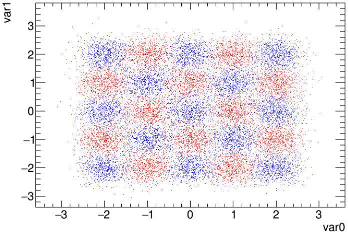
Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
```



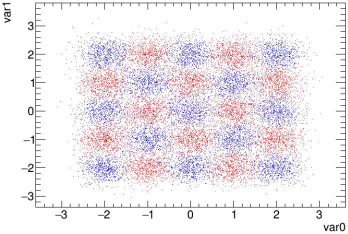
Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
```



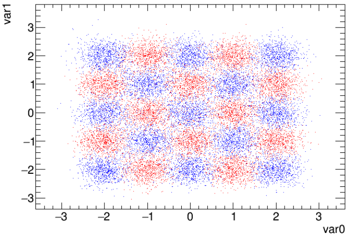
Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
    MinNodeSize=4%:MaxDepth=5:BoostType=AdaBoost:AdaBoostBeta=0.15:nCuts=80");
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
```



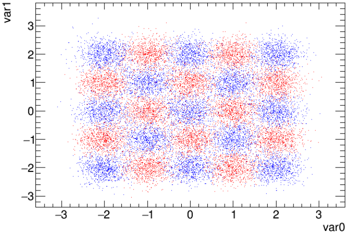
Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
    MinNodeSize=4%:MaxDepth=5:BoostType=AdaBoost:AdaBoostBeta=0.15:nCuts=80");
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
```



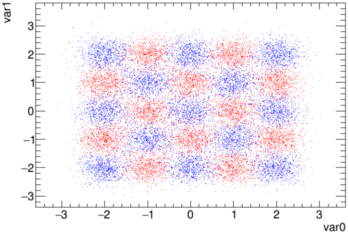
Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
    MinNodeSize=4%:MaxDepth=5:BoostType=AdaBoost:AdaBoostBeta=0.15:nCuts=80");
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
factory->TestAllMethods(); // Evaluate all MVAs using test events
```



Training with TMVA (Train.C)

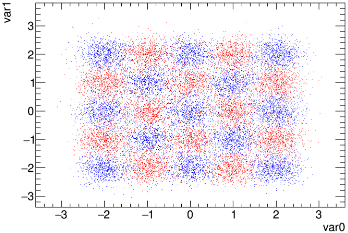
```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
```




```
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
    MinNodeSize=4%:MaxDepth=5:BoostType=AdaBoost:AdaBoostBeta=0.15:nCuts=80");
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
factory->TestAllMethods(); // Evaluate all MVAs using test events
// ----- Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
```

Training with TMVA (Train.C)

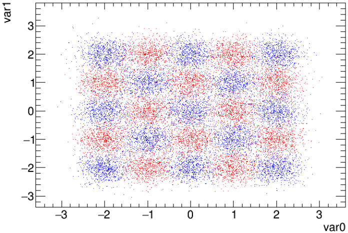
```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
```




```
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
    MinNodeSize=4%:MaxDepth=5:BoostType=AdaBoost:AdaBoostBeta=0.15:nCuts=80");
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
factory->TestAllMethods(); // Evaluate all MVAs using test events
// ----- Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
outputFile->Close();
delete factory; delete dataloader;
```

Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
TMVA::Factory *factory = new TMVA::Factory( "TMVAClassification", outputFile,
    "!V:Color:DrawProgressBar:Transformations=I:AnalysisType=Classification");
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
    MinNodeSize=4%:MaxDepth=5:BoostType=AdaBoost:AdaBoostBeta=0.15:nCuts=80");
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
factory->TestAllMethods(); // Evaluate all MVAs using test events
// ----- Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
outputFile->Close();
delete factory; delete dataloader;
```




```
TMVA::TMVAGui("output.root");
```

Apply classifier with TMVA (Apply.C)

```
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* data = (TTree*)inputFile->Get("TreeS");
Float_t var0=-99., var1=-99.;
data->SetBranchAddress("var0", &var0);
data->SetBranchAddress("var1", &var1);
```

Apply classifier with TMVA (Apply.C)

```
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* data = (TTree*)inputFile->Get("TreeS");
Float_t var0=-99., var1=-99.;
data->SetBranchAddress("var0", &var0);
data->SetBranchAddress("var1", &var1);
TMVA::Reader *reader = new TMVA::Reader();
reader->AddVariable( "var0", &var0 );
reader->AddVariable( "var1", &var1 );
```

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Float_t var0=-99., var1=-99.;
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TMVA::Reader *reader = new TMVA::Reader();
reader->AddVariable( "var0", &var0 );
reader->AddVariable( "var1", &var1 );
reader->BookMVA( "My BDT", "dataset/weights/TMVAClassification_BDT.weights.xml");
reader->BookMVA( "Fisher discriminant",
  "dataset/weights/TMVAClassification_Fisher.weights.xml");
```

Apply classifier with TMVA (Apply.C)

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TFile* inputFile = new TFile("dataSchachbrett.root");
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reader->BookMVA( "Fisher discriminant",
  "dataset/weights/TMVAClassification_Fisher.weights.xml");
// ------- start your event loop
for (Long64_t ievt=0; ievt<10; ++ievt) {
  data->GetEntry(ievt);
  double bdt = reader->EvaluateMVA("My BDT");
  double fisher = reader->EvaluateMVA("Fisher discriminant");
  cout<<"var0="<<var0<<" var1="<<var1<<" BDT="<<bdt<<" Fisher="<<fisher<<endl;
}
delete reader;
inputFile->Close();
```

Apply classifier with TMVA (Apply.C)

```
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* data = (TTree*)inputFile->Get("TreeS");
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  "dataset/weights/TMVAClassification_Fisher.weights.xml");
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  cout<<"var0="<<var0<<" var1="<<var1<<" BDT="<<bdt<<" Fisher="<<fisher<<endl;
}
delete reader;
inputFile->Close();
```

- More complete tutorial:
  - https://github.com/lmoneta/tmva-tutorial/tree/IML-tutorial-2018/tutorial_IML2018

Other boosting algorithms

ε-Boost (shrinkage)

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

ε-LogitBoost

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

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, GradientBoost, 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

Other averaging techniques

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Random forests

- Same as bagging
- In addition, pick random subset of variables to consider for each node split
- Two levels of randomisation, much more stable output

Other averaging techniques

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

Random forests

- Same as bagging
- In addition, pick random subset of variables to consider for each node split
- Two levels of randomisation, much more stable output

Trimming

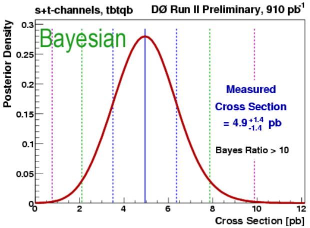
- Not exactly the same. Used to speed up training
- After some boosting, very few high weight events may contribute
- $\Rightarrow$ ignore events with too small a weight

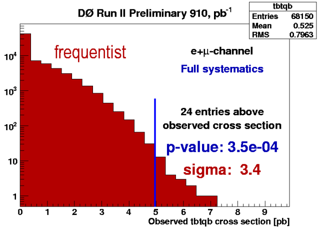
1 Introduction
2 Growing a tree
3 Tree (in)stability
4 Boosting
5 BDT performance
6 Concrete examples
7 Other averaging techniques
8 **BDTs in real physics cases**
9 BDT systematics
10 Software
11 Conclusion
12 References

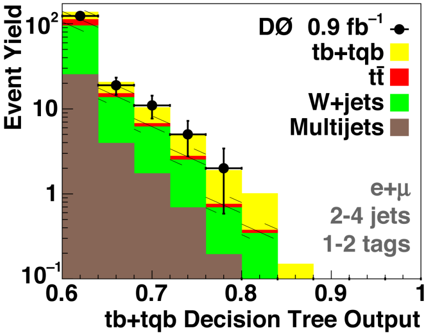
Single top production evidence at D0 (2006)

- Three multivariate techniques: BDT, Matrix Elements, BNN
- Most sensitive: BDT

$\sigma_{s+t} = 4.9 \pm 1.4$ pb
p-value = 0.035% (3.4σ)
SM compatibility: 11% (1.3σ)







$\sigma_s = 1.0 \pm 0.9$ pb
$\sigma_t = 4.2^{+1.8}_{-1.4}$ pb

Phys. Rev. D**78**, 012005 (2008)

Decision trees — 49 input variables

Object Kinematics

p_T(jet1)
p_T(jet2)
p_T(jet3)
p_T(jet4)
p_T(best1)
p_T(notbest1)
p_T(notbest2)
p_T(tag1)
p_T(untag1)
p_T(untag2)

Angular Correlations

ΔR(jet1,jet2)
cos(best1,lepton)$_{\mathrm{besttop}}$
cos(best1,notbest1)$_{\mathrm{besttop}}$
cos(tag1,alljets)$_{\mathrm{alljets}}$
cos(tag1,lepton)$_{\mathrm{btaggedtop}}$
cos(jet1,alljets)$_{\mathrm{alljets}}$
cos(jet1,lepton)$_{\mathrm{btaggedtop}}$
cos(jet2,alljets)$_{\mathrm{alljets}}$
cos(jet2,lepton)$_{\mathrm{btaggedtop}}$
cos(lepton,Q(lepton)$\times z$)$_{\mathrm{besttop}}$
cos(lepton$_{\mathrm{besttop}}$,besttop$_{\mathrm{CMframe}}$)
cos(lepton$_{\mathrm{btaggedtop}}$,btaggedtop$_{\mathrm{CMframe}}$)
cos(notbest,alljets)$_{\mathrm{alljets}}$
cos(notbest,lepton)$_{\mathrm{besttop}}$
cos(untag1,alljets)$_{\mathrm{alljets}}$
cos(untag1,lepton)$_{\mathrm{btaggedtop}}$

Event Kinematics

Aplanarity(alljets,W)
M(W,best1) ("best" top mass)
M(W,tag1) ("b-tagged" top mass)
H_T(alljets)
H_T(alljets$-$best1)
H_T(alljets$-$tag1)
H_T(alljets,W)
H_T(jet1,jet2)
H_T(jet1,jet2,W)
M(alljets)
M(alljets$-$best1)
M(alljets$-$tag1)
M(jet1,jet2)
M(jet1,jet2,W)
M_T(jet1,jet2)
M_T(W)
Missing E_T
p_T(alljets$-$best1)
p_T(alljets$-$tag1)
p_T(jet1,jet2)
Q(lepton)$\times\eta$(untag1)
$\sqrt{\hat{s}}$
Sphericity(alljets,W)

- Adding variables did not degrade performance
- Tested shorter lists, lost some sensitivity
- Same list used for all channels

Decision trees — 49 input variables

Object Kinematics

p_T(jet1)
p_T(jet2)
p_T(jet3)
p_T(jet4)
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p_T(notbest2)
p_T(tag1)
p_T(untag1)
p_T(untag2)

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ΔR(jet1,jet2)
cos(best1,lepton)$_{\text{besttop}}$
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cos(tag1,alljets)$_{\text{alljets}}$
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cos(jet1,alljets)$_{\text{alljets}}$
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cos(jet2,alljets)$_{\text{alljets}}$
cos(jet2,lepton)$_{\text{btaggedtop}}$
cos(lepton,Q(lepton)$\times z$)$_{\text{besttop}}$
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cos(notbest,alljets)$_{\text{alljets}}$
cos(notbest,lepton)$_{\text{besttop}}$
cos(untag1,alljets)$_{\text{alljets}}$
cos(untag1,lepton)$_{\text{btaggedtop}}$

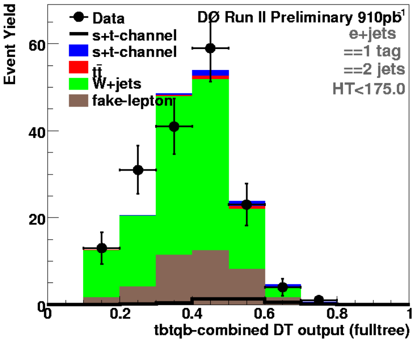
Event Kinematics

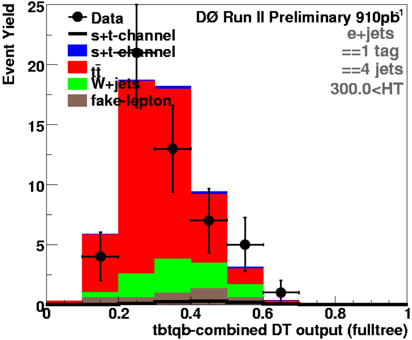
Aplanarity(alljets,W)
M(W,best1) ("best" top mass)
M(W,tag1) ("b-tagged" top mass)
H_T(alljets)
H_T(alljets−best1)
H_T(alljets−tag1)
H_T(alljets,W)
H_T(jet1,jet2)
H_T(jet1,jet2,W)
M(alljets)
M(alljets−best1)
M(alljets−tag1)
M(jet1,jet2)
M(jet1,jet2,W)
M_T(jet1,jet2)
M_T(W)
Missing E_T
p_T(alljets−best1)
p_T(alljets−tag1)
p_T(jet1,jet2)
Q(lepton)$\times\eta$(untag1)
$\sqrt{\hat{s}}$
Sphericity(alljets,W)

- Adding variables did not degrade performance
- Tested shorter lists, lost some sensitivity
- Same list used for all channels
- Best theoretical variable: H_T(alljets,W). But detector not perfect $\Rightarrow$ capture the essence from several variations usually helps "dumb" MVA

- Validate method on data in no-signal region

- **"W+jets":** $= 2$ jets, $H_T(\text{lepton},\not{E}_T,\text{alljets}) < 175$ GeV
- **"ttbar":** $= 4$ jets, $H_T(\text{lepton},\not{E}_T,\text{alljets}) > 300$ GeV

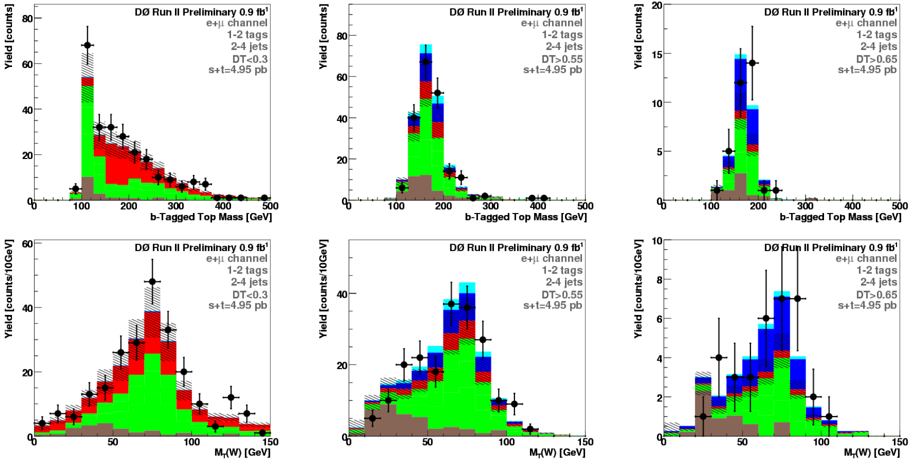




- Good agreement

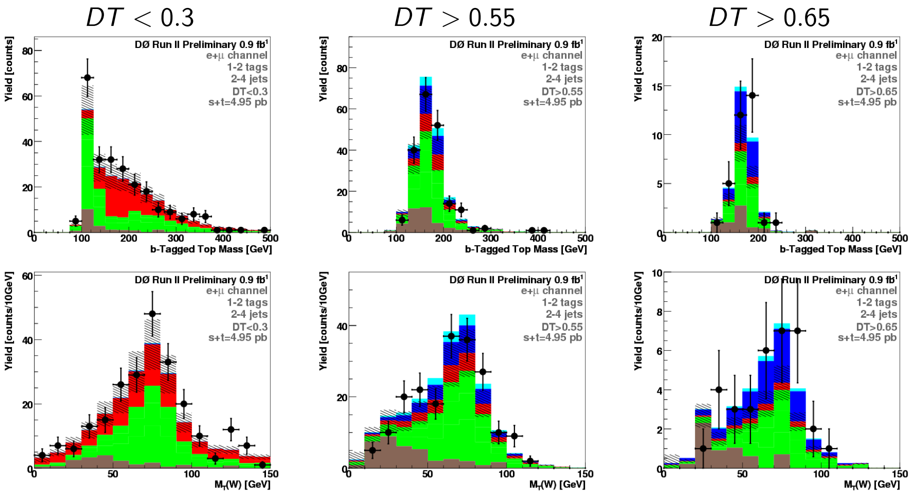
Boosted decision tree event characteristics

$DT < 0.3$ $\quad$ $DT > 0.55$ $\quad$ $DT > 0.65$



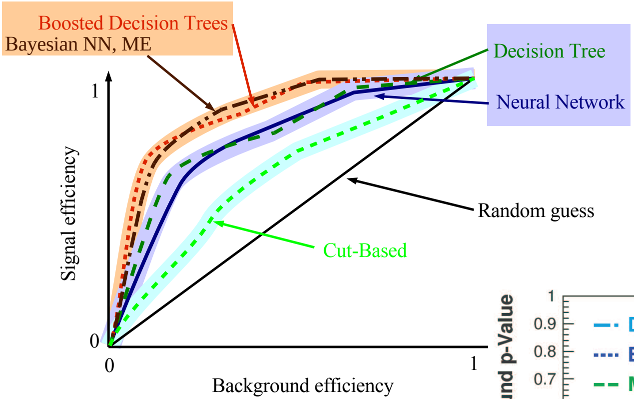
- High BDT region = shows masses of real t and W $\Rightarrow$ expected
- Low BDT region = background-like $\Rightarrow$ expected

Boosted decision tree event characteristics



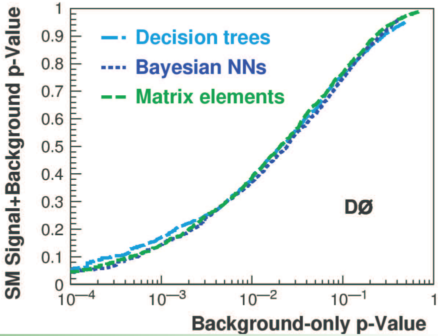
- High BDT region = shows masses of real t and W ⇒ expected
- Low BDT region = background-like ⇒ expected
- Above does NOT tell analysis is ok, but not seeing this could be a sign of a problem

Comparison for D0 single top evidence



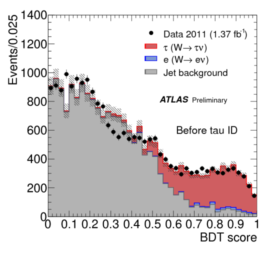
- Cannot know *a priori* which method will work best
- ⇒ Need to experiment with different techniques

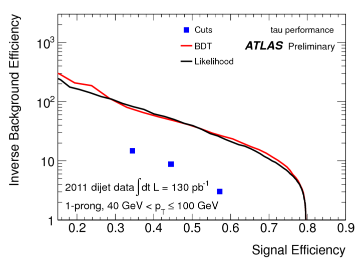
Power curve



ATLAS tau identification

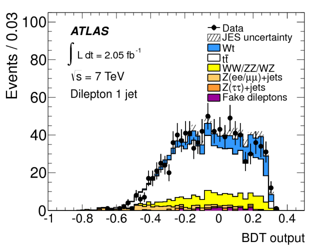
- Now used both offline and online
- Systematics: propagate various detector/theory effects to BDT output and measure variation





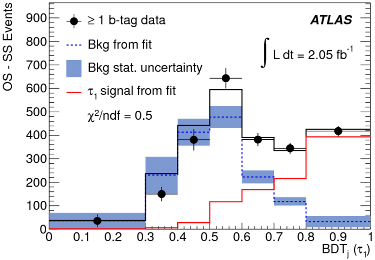
ATLAS Wt production evidence

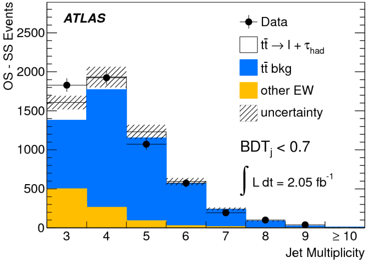
- Phys.Lett. B716 (2012) 142-159
- BDT output used in final fit to measure cross section
- Constraints on systematics from profiling

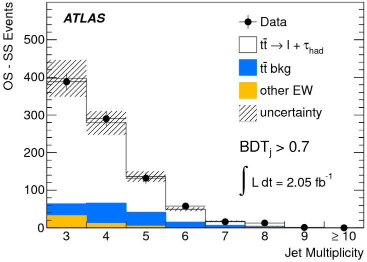


Phys.Lett. B717 (2012) 89-108

- BDT for tau ID: one to reject electrons, one against jets
- Fit BDT output to get tau contribution in data





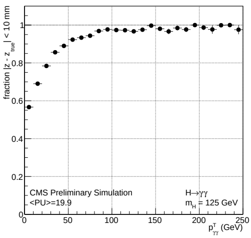


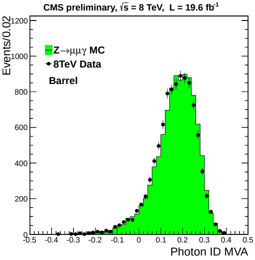
BDT in HEP: CMS $H \to \gamma\gamma$ result

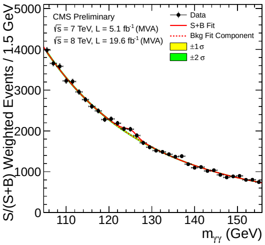
CMS-PAS-HIG-13-001

Hard to use more BDT in an analysis:

- vertex selected with BDT
- 2^{nd} vertex BDT to estimate probability to be within 1cm of interaction point
- photon ID with BDT
- photon energy corrected with BDT regression
- event-by-event energy uncertainty from another BDT
- several BDT to extract signal in different categories



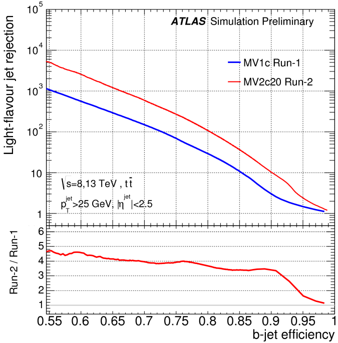


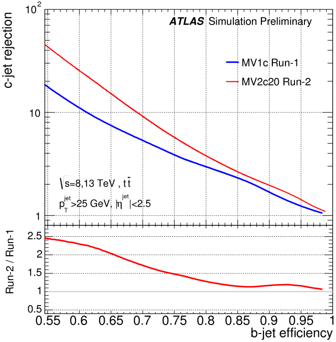


BDT in HEP: ATLAS b-tagging in Run 2

ATL-PHYS-PUB-2015-022

- Run 1 MV1c: NN trained from output of other taggers
- Run 2 MV2c20: BDT using feature variables of underlying algorithms (impact parameter, secondary vertices) and p_T, η of jets
- Run 2: introduced IBL (new innermost pixel layer)
  $\Rightarrow$ explains part of the performance gain, but not all

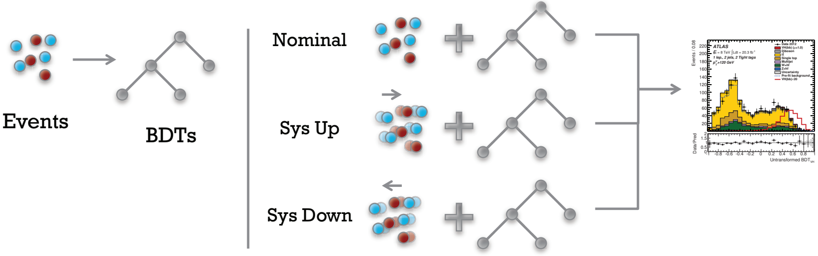




BDT and systematics

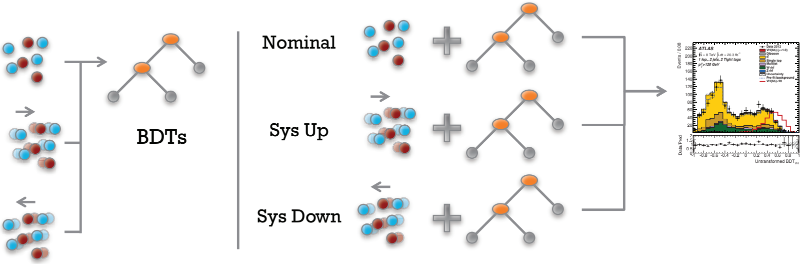
- No particular rule
- BDT output can be considered as any other cut variable (just more powerful). Evaluate systematics by:
  - varying cut value
  - retraining
  - calibrating, etc.
- Most common (and appropriate, I think): propagate other uncertainties (detector, theory, etc.) up to BDT ouput and check how much the analysis is affected
- More and more common: profiling.
  Watch out:
  - BDT output powerful
  - signal region (high BDT output) probably low statistics
    $\Rightarrow$ potential recipe for disaster if modelling is not good
- May require extra systematics, not so much on technique itself, but because it probes specific corners of phase space and/or wider parameter space (usually loosening pre-BDT selection cuts)

BDT and systematics



S. Hageböck

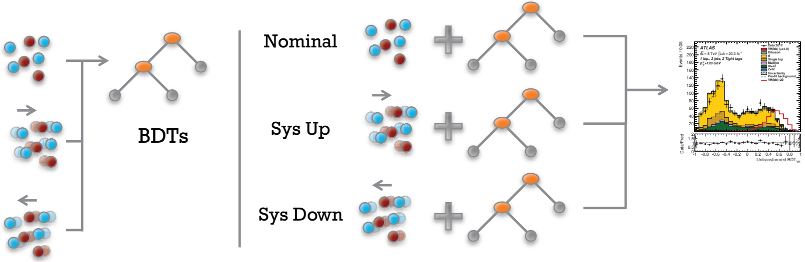
BDT and systematics



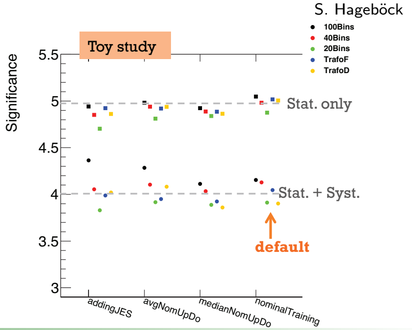
S. Hageböck

- Hope: seeing systematics-affected events during training may make the BDT less sensitive to systematic effects

BDT and systematics



- Hope: seeing systematics-affected events during training may make the BDT less sensitive to systematic effects



Boosted decision tree software

- Go for a fully integrated solution
  - use different multivariate techniques easily
  - spend your time on understanding your data and model
- Examples:
  - Weka. Written in Java, open source, very good published manual. Not written for HEP but very complete ▸ http://www.cs.waikato.ac.nz/ml/weka/
  - StatPatternRecognition ▸ http://statpatrec.sourceforge.net/
  - *T*MVA (Toolkit for MultiVariate Analysis) Integrated in ROOT, complete manual ▸ http://tmva.sourceforge.net
  - scikit-learn (python) [see G. Louppe's tutorial] ▸ http://scikit-learn.org
  - pylearn2 (python) ▸ https://github.com/lisa-lab/pylearn2
- Dedicated to BDT: XGBoost ▸ arXiv:1603.02754 ▸ https://github.com/dmlc/xgboost

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)
- Has become rather fashionable in HEP
- Possibly soon overpowered by deep learning algorithms, although trickier to optimise
- Whichever technique you use, expect a lot of scepticism: you will 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. But DO NOT show them useless plots like BDT output on training and testing, please!
- As with other advanced techniques,
  no point in using them if data are not understood and well modelled

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BACKUP

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

Pruning a tree I

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 II: 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 III: 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