Boosted decision trees

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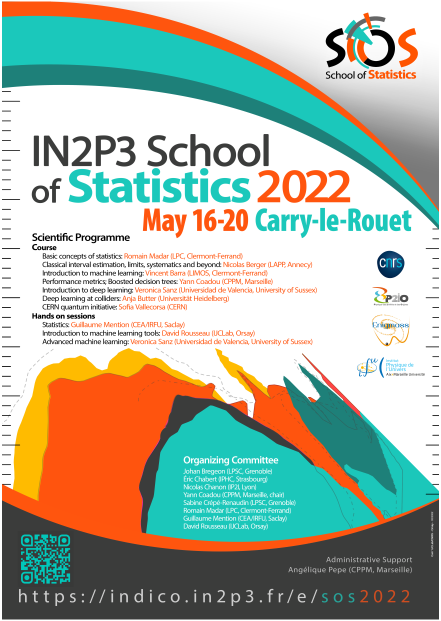

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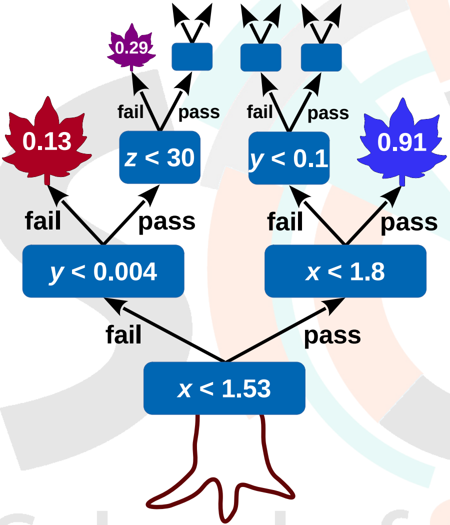

1. **Decision trees**
   - Algorithm
   - Tree hyperparameters
   - Splitting a node
   - Variable selection

Introduction

Decision tree origin

- Machine-learning technique, widely used in social sciences.
  Originally data mining/pattern recognition, then medical diagnosis, 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

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 (min leaf size, max tree depth, insufficient improvement, perfect classification, etc.)
- 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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    - $p_\mathrm{T} < 56$ GeV, separation $= 3$
    - $H_\mathrm{T} < 242$ GeV, separation $= 5$
    - $M_t < 105$ GeV, separation $= 0.7$

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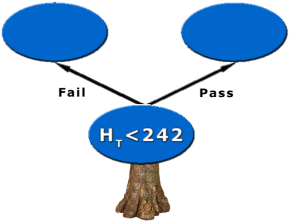

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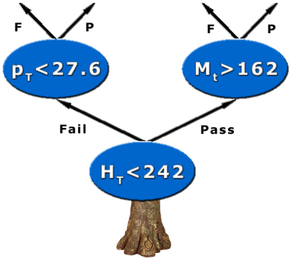

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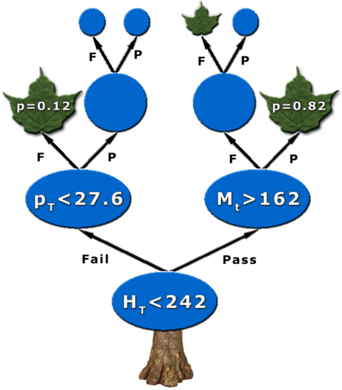
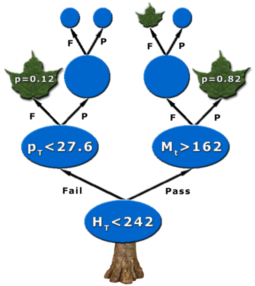
- Repeat recursively on each node
- Splitting stops: e.g. events with $H_\mathrm{T} < 242$ GeV and $M_t > 162$ GeV are signal like ($p = 0.82$)



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 $\left(\frac{s}{s+b}\text{, with weighted events}\right)$ 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 $H_\mathrm{T} < 242$ 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

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

Selection of splits

- list of questions ($variable_i < cut_i$?, "Is jet b-tagged?")
- 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

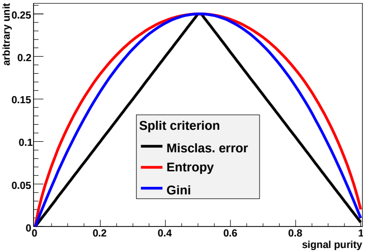
Splitting a node

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 $\Delta i(s^*, t) = \max_{s\in\{\text{splits}\}} \Delta i(s,t)$
- Maximising $\Delta i(s,t) \equiv$ minimising overall tree impurity

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 $(-\frac{s^2}{b})$

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
- 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

Transforming input variables

- Completely insensitive to replacement of any subset of input variables by (possibly different) arbitrary strictly monotone functions of them (same order $\Rightarrow$ same DT):
  - 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 II

Transforming input variables

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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 (mean decrease impurity MDI)

- 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

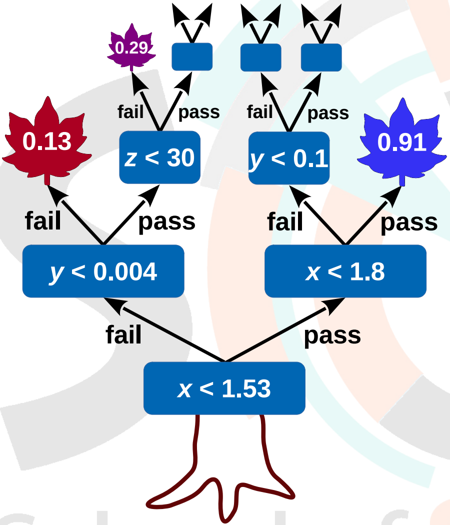
- x_j may be just a little worse than x_i but will never be picked
- x_j is ranked as irrelevant
- But remove x_i and x_j becomes very relevant
  $\Rightarrow$ careful with interpreting ranking (specific to training)

Permutation importance (mean decrease accuracy MDA)

- Applicable to any already trained classifier
- Randomly shuffle each variable in turn and measure decrease of performance
- Important variable $\Rightarrow$ big loss of performance
- Can also be performed on validation sample
- Beware of correlations

Choosing variables

- Usually try to have as few variables as possible
- But difficult: correlations, possibly large number to consider, large phase space with different properties in different regions
- *Brute force:* with n variables train all n, $n-1$, etc. combinations, pick best
- *Backward elimination:* train with n variables, then train all $n-1$ variables trees and pick best one; now train all $n-2$ variables trees starting from the $n-1$ variable list; etc. Pick optimal cost-complexity tree.
- *Forward greedy selection:* start with $k=1$ variable, then train all $k+1$ variables trees and pick the best; move to $k+2$ variables; etc.



2 Limitations

- Training sample composition
- Pruning a tree
- Ensemble learning

Tree instability: training sample composition

- Small changes in sample can lead to very different tree structures (high variance)
- 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

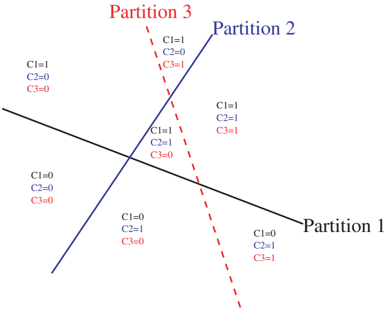
Why prune a tree?

- 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)

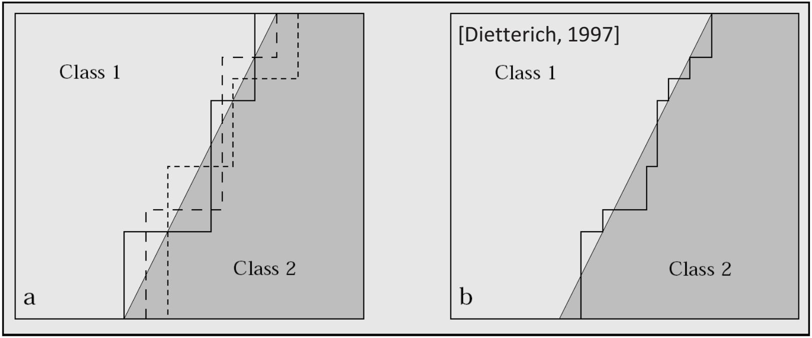
- Pre-pruning (early stopping condition like min leaf size, max depth)
- Expected error pruning (based on statistical error estimate)
- Cost-complexity pruning (penalise "complex" trees with many nodes/leaves)

- 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



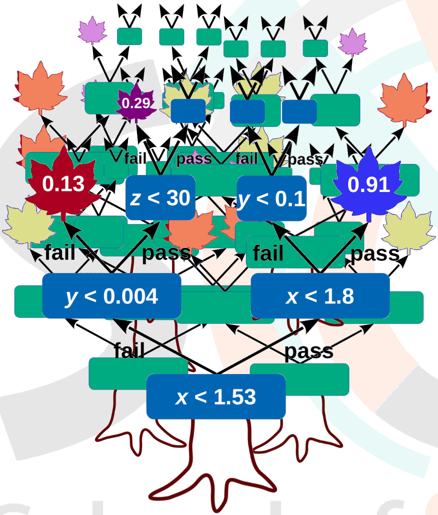
Tree (in)stability solution: averaging

- 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: ensemble learning

Boosted decision trees



3 Boosted decision trees

- Introduction
- AdaBoost
- Figures of merit
- Clues to boosting performance
- Gradient boosting
- Other averaging techniques
- Performance examples
- BDT usage in HEP

Boosting: a brief history

First provable algorithm [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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Then

- Variation [Freund 1995]: boost by majority (combining many learners with fixed error rate)
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When it really picked up in HEP

- MiniBooNe compared performance of different boosting algorithms and neural networks for particle ID [MiniBooNe 2005]
- D0 claimed first evidence for single top quark production [D0 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

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
- 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 $\mathbb{T}_{k+1}$:

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

- 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 error rate

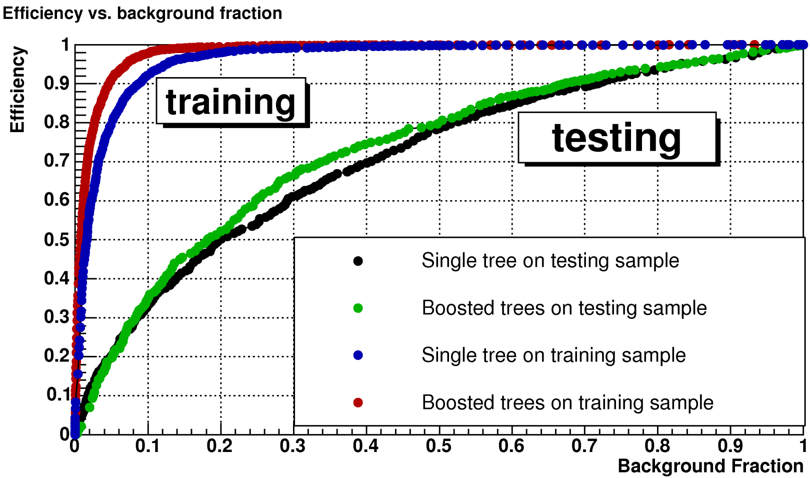
Misclassification rate ε on training sample

- 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 overfitted

Overtraining?

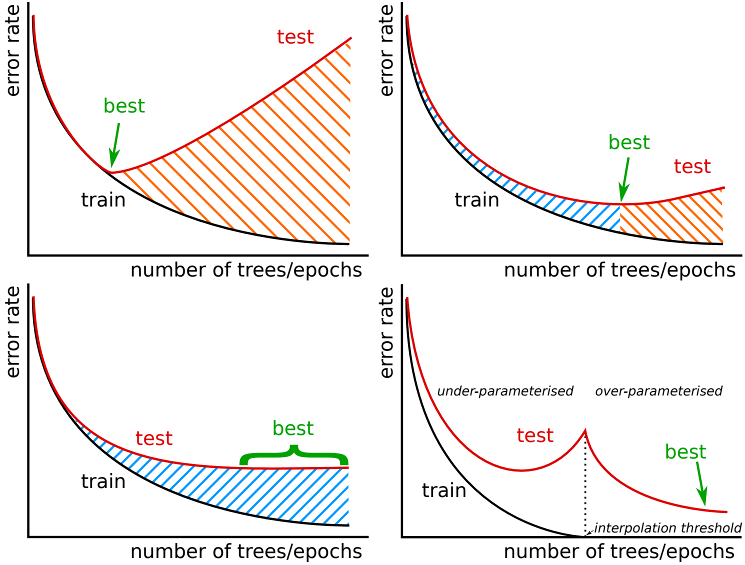
- Error rate on test sample may reach a minimum and then potentially rise. Stop boosting at the minimum.
- In principle AdaBoost *must* overfit training sample
- In many cases in literature, no loss of performance due to overtraining
  - may have to do with fact that successive trees get in general smaller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

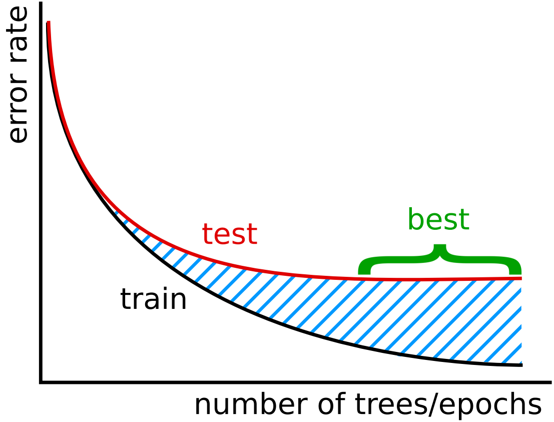
Overtraining estimation: good or bad?



"bad" overtraining (overfitting) / "good" overtraining (still underfitting)

Overtraining estimation: good or bad?

- Typical situation for boosted decision trees

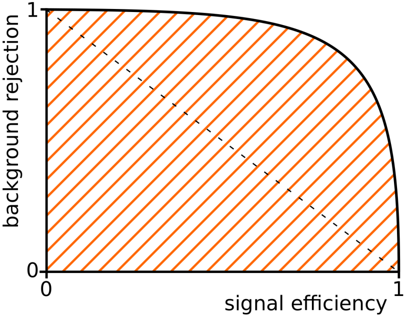


"bad" overtraining (overfitting) / "good" overtraining (still underfitting)

Figures of merit

- Common in ML: accuracy = fraction of correctly classified samples
  - not appropriate with imbalanced classes

- Receiver operating characteristic (ROC)
  - true positive rate vs. false positive rate
  - ...or equivalently signal efficiency vs background efficiency
  - can also replace bkg efficiency by bkg rejection (1−bkg efficiency)
  - Measure: area under the curve (AUC)



- Excess significance $s/\sqrt{b}$ and cross-section significance $s/\sqrt{s+b}$

Figures of merit

- Better: approximate median significance ($\approx s/\sqrt{b}$ for $s \ll b$):

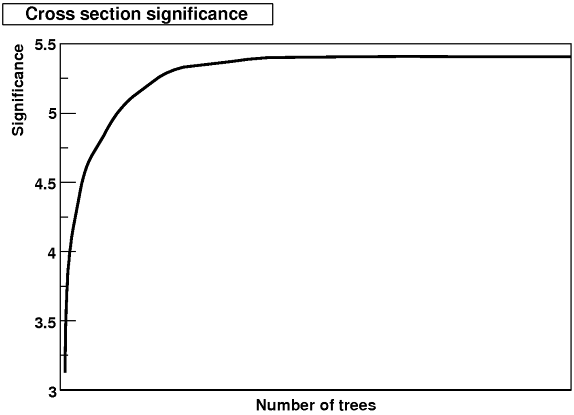
$$\mathrm{AMS} = \sqrt{2\left((s+b)\ln\left(1+\frac{s}{b}\right)-s\right)}$$

- Adding background uncertainty $b \to b \pm \sigma$ (observing n):

$$Z = \begin{cases} +\sqrt{2\left(n\ln\left[\frac{n(b+\sigma^2)}{b^2+n\sigma^2}\right]-\frac{b^2}{\sigma^2}\ln\left[1+\frac{\sigma^2(n-b)}{b(b+\sigma^2)}\right]\right)} & \text{if } n \geqslant b \\ -\sqrt{2\left(n\ln\left[\frac{n(b+\sigma^2)}{b^2+n\sigma^2}\right]-\frac{b^2}{\sigma^2}\ln\left[1+\frac{\sigma^2(n-b)}{b(b+\sigma^2)}\right]\right)} & \text{if } n < b \end{cases}$$

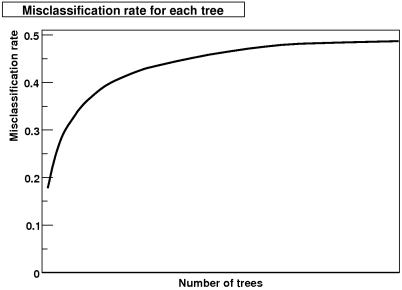
  - simplifies to AMS for vanishing uncertainty ($\sigma = 0$)
  - recommended by ATLAS collaboration ATL-PHYS-PUB-2020-025
- Simplifies to $s/\sqrt{b+\sigma^2}$ for $s \ll b$
- Many more metrics, see e.g. in scikit-learn documentation

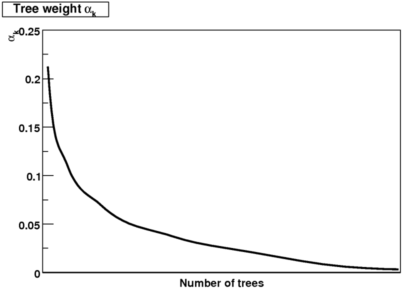
Cross section significance ($s/\sqrt{s+b}$)



- 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
- But adding trees may increase reliability of prediction: margins explanation [Shapire&Freund 2012]
- Double descent risk curve and interpolation regime [Belkin 2019]

Gradient boosting [Friedman 2001]

- AdaBoost recast in a statistical framework: corresponds to minimising an exponential loss
- Generalisation: formulate boosting as numerical optimisation problem, minimise loss function by adding trees using gradient descent procedure
- Procedure:
  - Build imperfect model F_k at step k (sometimes $F_k(x) \neq y$)
  - Improve model: $F_{k+1}(x) = F_k(x) + h_k(x) = y$, or residual $h_k(x) = y - F_k(x)$
  - Train new classifier on residual
- Example: mean squared error loss function $L_{\mathrm{MSE}}(x, y) = \frac{1}{2}\left(y - F_k(x)\right)^2$
  - minimising loss $J = \sum_i L_{\mathrm{MSE}}(x_i, y_i)$ leads to $\frac{\partial J}{\partial F_k(x_i)} = F_k(x_i) - y_i$
    $\Rightarrow$ residual as negative gradient: $h_k(x_i) = y_i - F_k(x_i) = -\frac{\partial J}{\partial F_k(x_i)}$
- Generalised to any differentiable loss function

Other averaging techniques

Bagging (Bootstrap aggregating) [Breiman 1996]

- 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
- Applicable to other techniques than DT
  - tends to produce more stable and better classifier

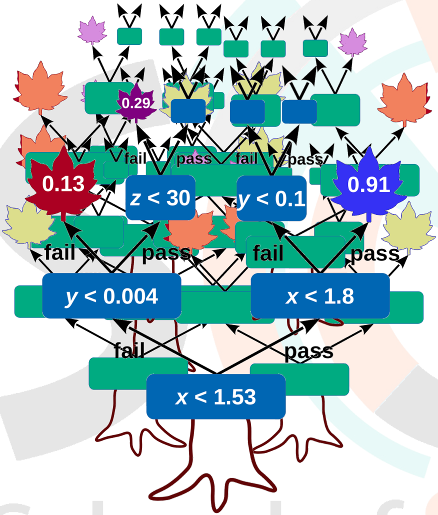
Other averaging techniques

Bagging (Bootstrap aggregating) [Breiman 1996]

- 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
- Applicable to other techniques than DT
  - tends to produce more stable and better classifier

Random forests [Breiman 2001]

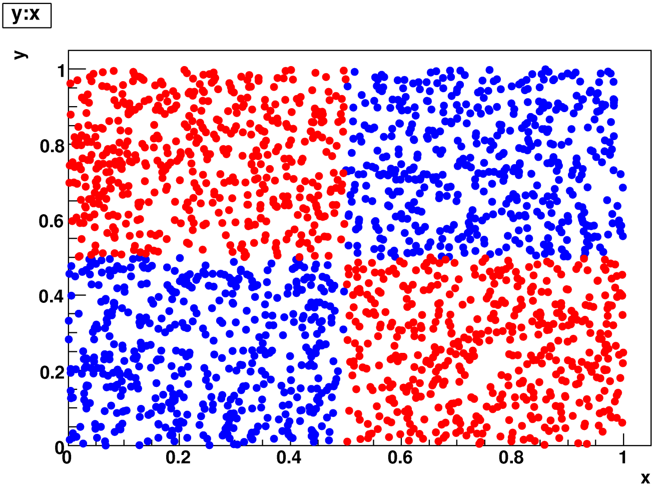
- Same as bagging
- In addition, pick random subset of variables to consider for each node split
- Two levels of randomisation, much more stable output
- Often as good as boosting



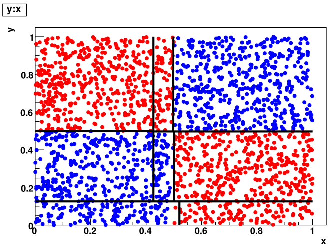
3 Boosted decision trees

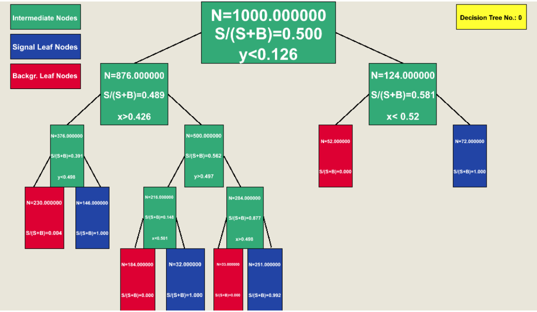
- Performance examples
  - XOR problem
  - Boosting longer
  - Many small trees or fewer large trees?

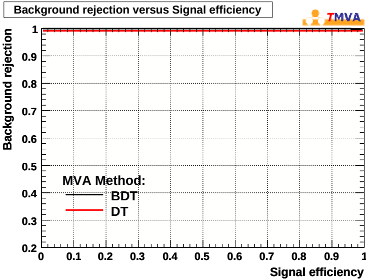
Example: XOR problem



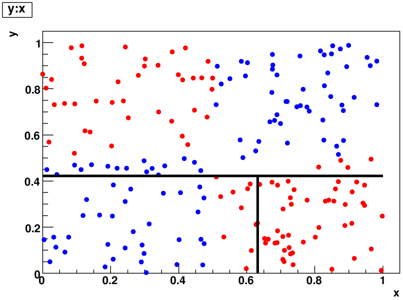
Example: XOR problem

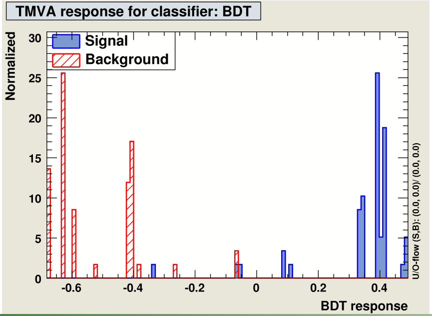






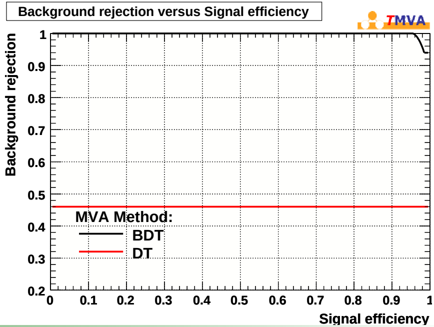
Example: XOR with 100 events



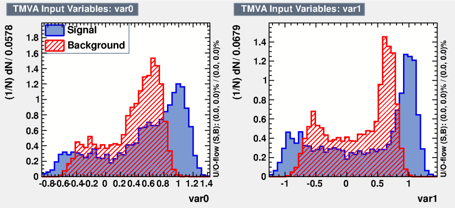


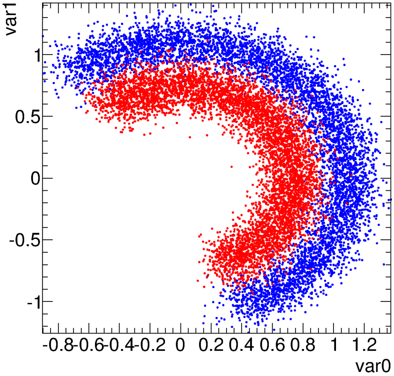
Small statistics

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



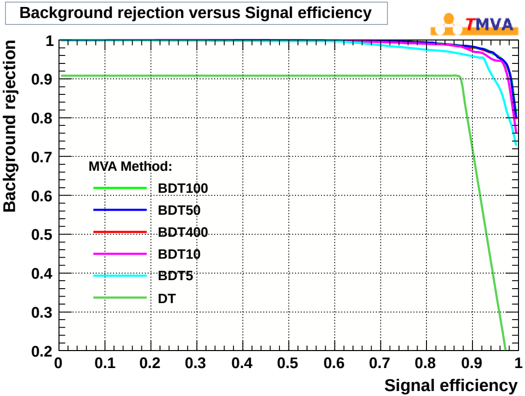
Example dataset





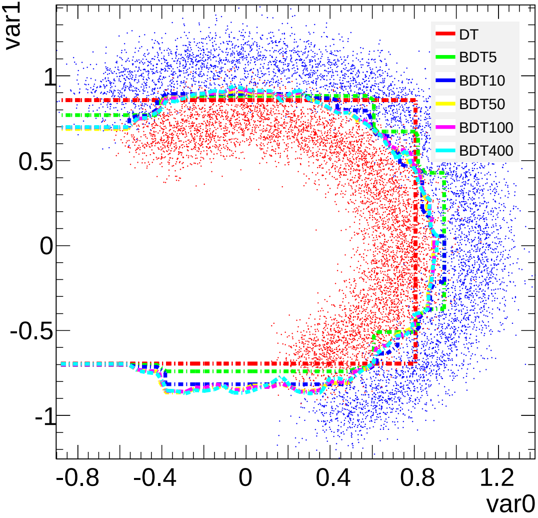
Boosting longer

- Compare performance of single DT and BDT with more and more trees (5 to 400)
- All other parameters unchanged



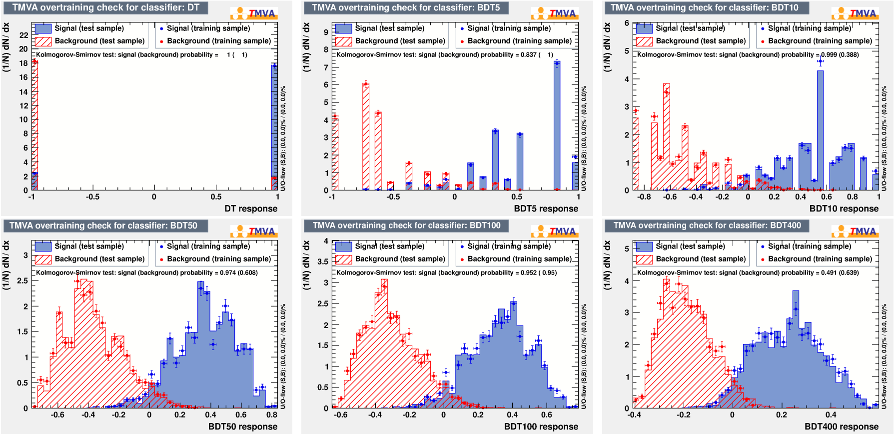
- Single (small) DT: not so good
- More trees $\Rightarrow$ improve performance until saturation

Decision contours



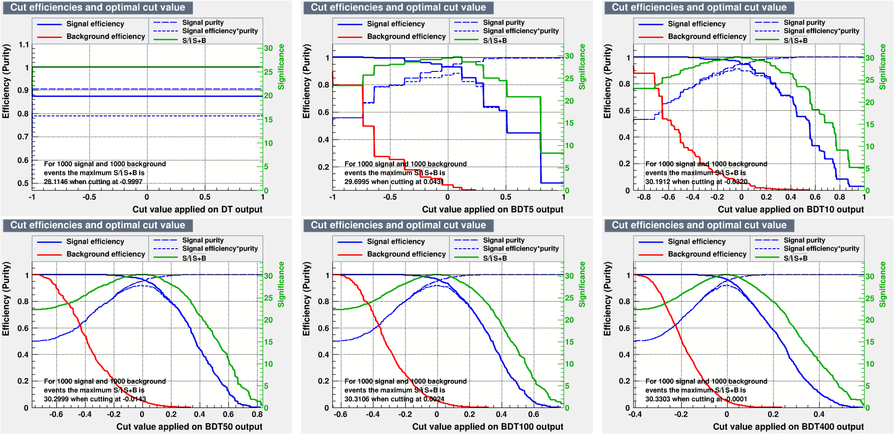
- Note: max tree depth = 3
- Single (small) DT: not so good. Note: a larger tree would solve this problem
- More trees ⇒ improve performance (less step-like, closer to optimal separation) until saturation
- Largest BDTs: wiggle a little around the contour ⇒ picked up features of training sample, that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

Training/testing output



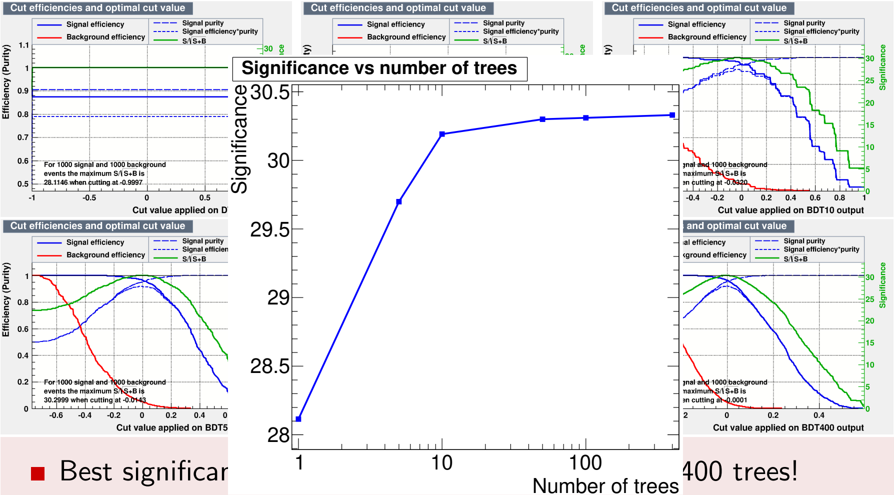
- Better shape with more trees: quasi-continuous
- Overtraining because of disagreement between training and testing? Let's see...

Performance in optimal significance



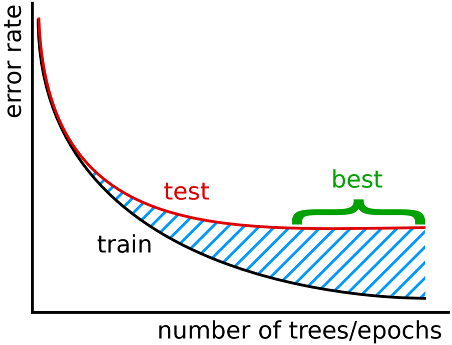
- Best significance actually obtained with last BDT, 400 trees!
- But to be fair, equivalent performance with 10 trees already
- Less "stepped" output desirable? ⇒ maybe 50 is reasonable

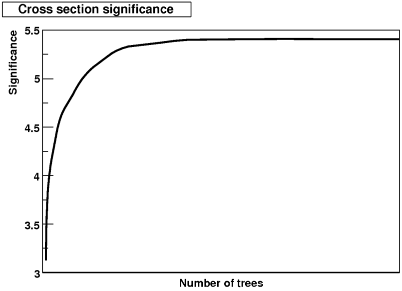
Performance in optimal significance



- Best significan... 400 trees!
- But to be fair, equivalent performance with 10 trees already
- Less "stepped" output desirable? ⇒ maybe 50 is reasonable

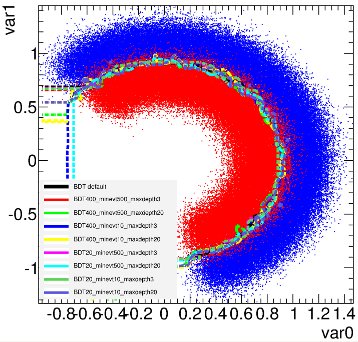
Getting best performance

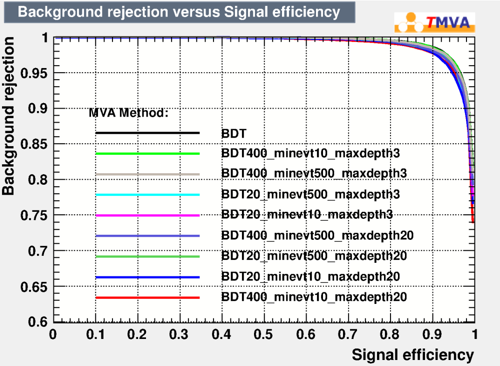




Many small trees or fewer large trees?

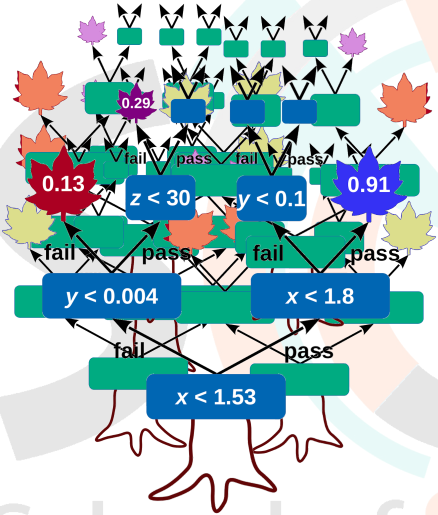
- Generating larger dataset to avoid stats limitations
- 20 or 400 trees; minimum leaf size: 10 or 500 events
- Maximum depth (max # of cuts to reach leaf): 3 or 20





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

BDT usage in HEP



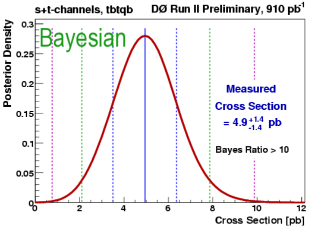
3 Boosted decision trees

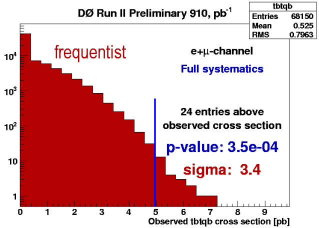
- BDT usage in HEP
  - Single top search at D0
  - LHC examples
  - BDT and systematics

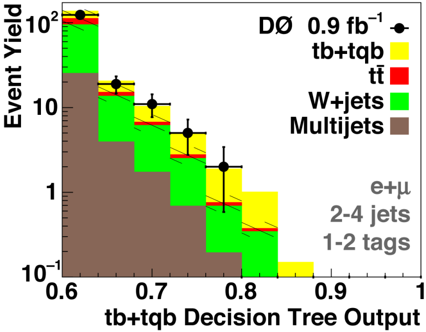
Single top production evidence at D0 (2006)

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

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







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

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

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

Event Kinematics

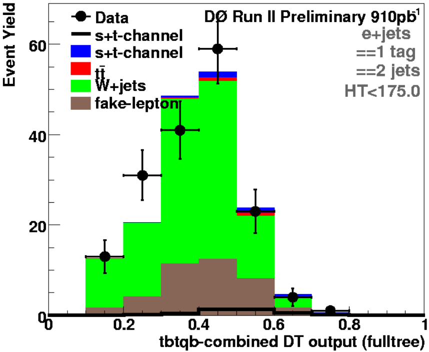
Aplanarity(alljets,W)
M(W,best1) ("best" top mass)
M(W,tag1) ("b-tagged" top mass)
H_T(alljets)
H_T(alljets$-$best1)
H_T(alljets$-$tag1)
H_T(alljets,W)
H_T(jet1,jet2)
H_T(jet1,jet2,W)
M(alljets)
M(alljets$-$best1)
M(alljets$-$tag1)
M(jet1,jet2)
M(jet1,jet2,W)
M_T(jet1,jet2)
M_T(W)
Missing E_T
p_T(alljets$-$best1)
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

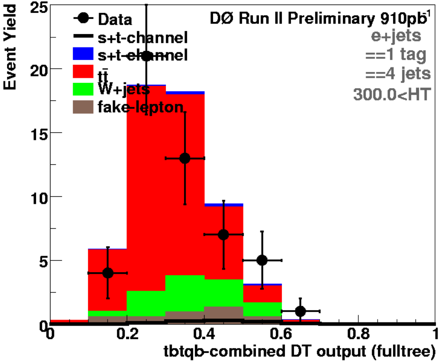
Cross-check samples

- Validate method on data in no-signal region

- **"W+jets":** $= 2$ jets, H_T(lepton,E_T^{miss},alljets) < 175 GeV



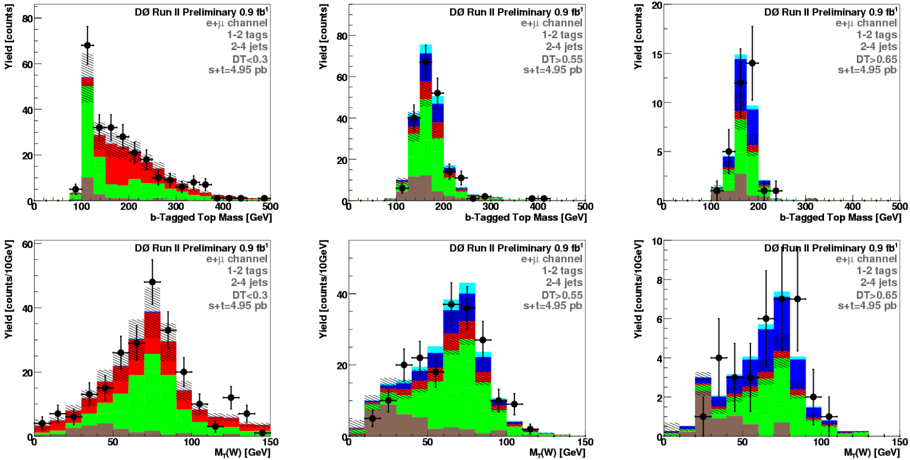
- **"ttbar":** $= 4$ jets, H_T(lepton,E_T^{miss},alljets) > 300 GeV



- Good agreement

Boosted decision tree event characteristics

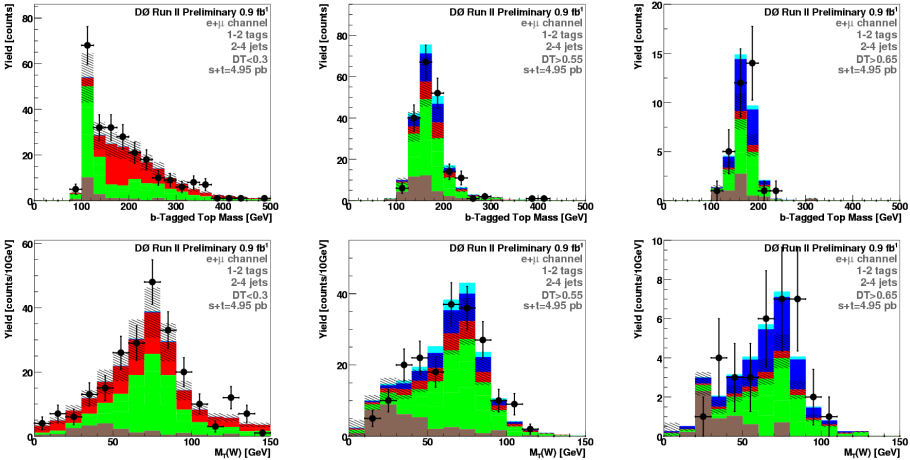
$DT < 0.3$ | $DT > 0.55$ | $DT > 0.65$



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

Boosted decision tree event characteristics

$DT < 0.3$ $DT > 0.55$ $DT > 0.65$



- 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

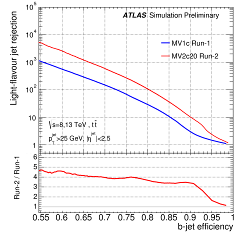
BDT in HEP

ATLAS b-tagging in Run 2

‣ Eur. Phys. J. C 79 (2019) 970

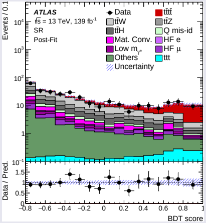
- Run 1 MV1c: NN trained from output of other taggers
- Run 2 MV2c20: BDT using feature variables of underlying algorithms and p_{T}, η of jets
- Run 2: introduced IBL (new innermost pixel layer)

  $\Rightarrow$ explains part of the performance gain, but not all



ATLAS $t\bar{t}t\bar{t}$ production evidence

- ‣ Eur. Phys. J. C **80** (2020) 1085 ‣ arXiv:2007.14858 [hep-ex]
- BDT output used in final fit to measure cross section
- Constraints on systematic uncertainties from profiling

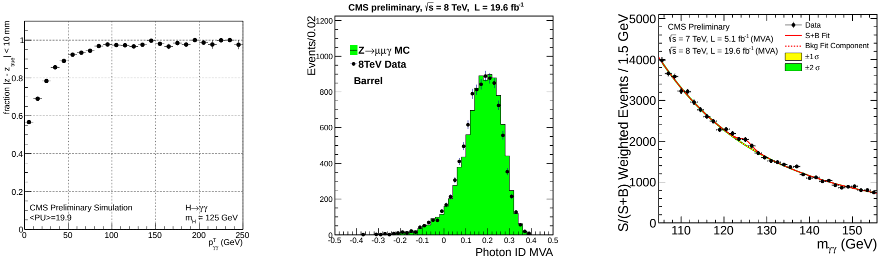


BDT in HEP: CMS $H \to \gamma\gamma$ result

▸ CMS-PAS-HIG-13-001

Hard to use more BDT in an analysis:

- vertex selected with BDT
- 2nd 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

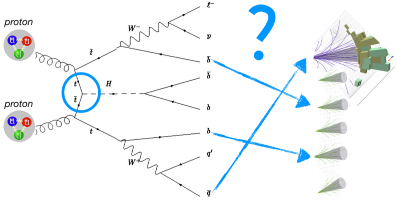


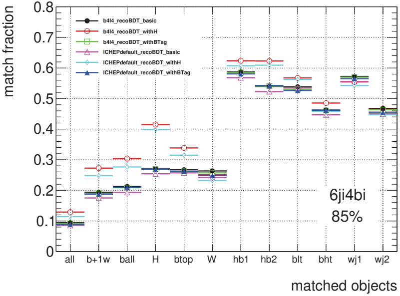
BDT in HEP: reducing combinatorics

$t\bar{t}H(b\bar{b})$ reconstruction

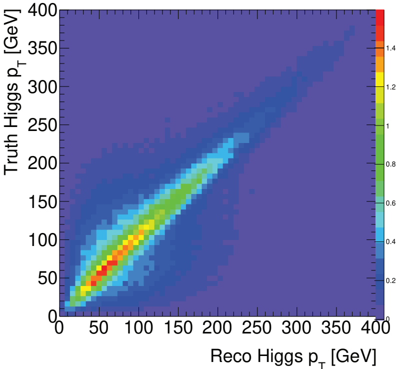
- Match jets and partons in high-multiplicity final state
- BDT trained on all combinations
- New inputs to classification BDT
- Access to Higgs p_T, origin of b-jets

▸ Phys. Rev. D 97, 072016 (2018) ▸ arXiv:2111.06712 [hep-ex]





▸ thesis

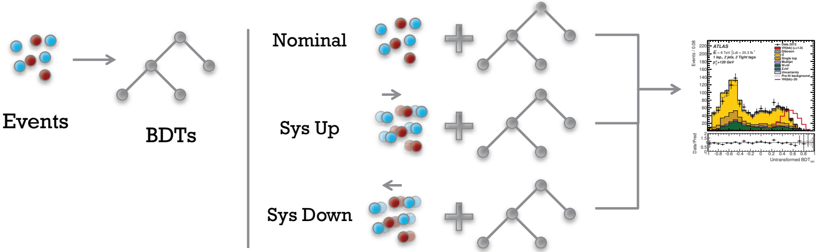


▸ thesis

BDT and systematics

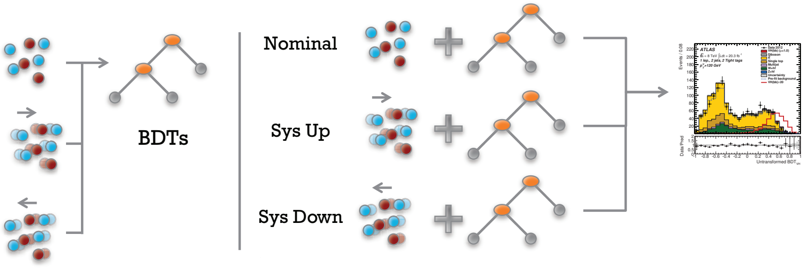
- No particular rule
- BDT output can be considered as any other cut variable (just more powerful). Evaluate systematics by:
  - varying cut value
  - retraining
  - calibrating, etc.
- Most common (and appropriate): propagate other uncertainties (detector, theory, etc.) up to BDT ouput and check how 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

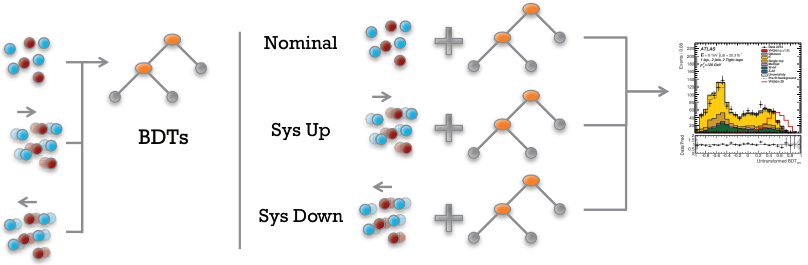
BDT and systematics



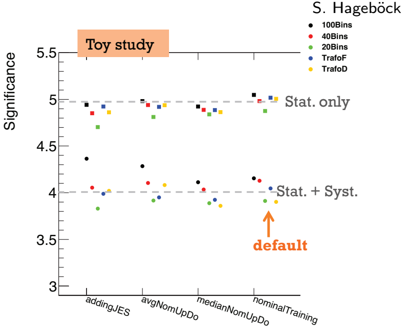
S. Hageböck

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

BDT and systematics



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



Decision trees are not dead! e.g. NeurIPS2019

- PIDForest: Anomaly Detection via Partial Identification ▸ NeurIPS
- A Debiased MDI (Mean Decrease of Impurity) Feature Importance Measure for Random Forests ▸ NeurIPS
- MonoForest framework for tree ensemble analysis ▸ NeurIPS
- Faster Boosting with Smaller Memory (Yoav S Freund) ▸ NeurIPS
- Minimal Variance Sampling in Stochastic Gradient Boosting ▸ NeurIPS
- Regularized Gradient Boosting ▸ NeurIPS
- Partitioning Structure Learning for Segmented Linear Regression Trees ▸ NeurIPS
- Random Tessellation Forests ▸ NeurIPS
- Optimal Sparse Decision Trees ▸ NeurIPS
- Provably robust boosted decision stumps and trees against adversarial attacks ▸ NeurIPS
- Robustness Verification of Tree-based Models ▸ NeurIPS

NEURAL INFORMATION PROCESSING SYSTEMS

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:
  - **TMVA** (Toolkit for MultiVariate Analysis)
    Integrated in ROOT, complete manual ‣ https://root.cern/tmva
  - scikit-learn (python) ‣ http://scikit-learn.org
- Dedicated to BDT (python):
  - XGBoost (popular in HEP) ‣ arXiv:1603.02754 ‣ https://github.com/dmlc/xgboost
    (note: cannot handle negative weights)
  - LightGBM (Microsoft) ‣ https://lightgbm.readthedocs.io
  - CatBoost (Yandex) ‣ https://catboost.ai/

Conclusion

- Decision trees: natural extension to cut-based analysis
- Greatly improved performance with boosting (and also with bagging, random forests)
- Very common in HEP results (soon has-been?)
  - often using TMVA in ROOT or python (see backup)
  - more and more with XGBoost, LightGBM, etc. (see hands-on)
- 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 yourself and others that your advanced technique leads to meaningful and reliable results

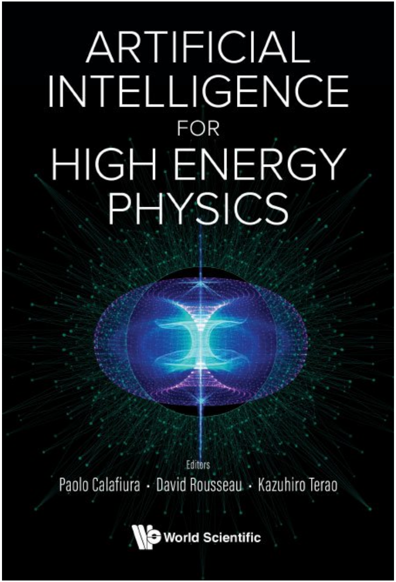
  ⇒ ensemble tests, use several techniques, compare to random grid search, etc. But DO NOT show them useless plots like BDT output on training and testing to measure overtraining, please!
- As with other advanced techniques,

  no point in using them if data are not understood and well modelled

Brand new reference book (March 2022)

Artificial Intelligence for High Energy Physics

https://doi.org/10.1142/12200



Contents:

- L. Breiman, J.H. Friedman, R.A. Olshen and C.J. Stone, *Classification and Regression Trees*, Wadsworth, Stamford, 1984
- R.E. Schapire, "The strength of weak learnability" ▸ Machine Learning **5** (1990) 197
- Y. Freund, "Boosting a weak learning algorithm by majority" ▸ Information and computation **121** (1995) 256
- Y. Freund and R.E. Schapire, "Experiments with a New Boosting Algorithm" in *Machine Learning: Proceedings of the Thirteenth International Conference*, edited by L. Saitta (Morgan Kaufmann, San Fransisco, 1996) p. 148
- Y. Freund and R.E. Schapire, "A short introduction to boosting" ▸ Journal of Japanese Society for Artificial Intelligence 14 (1999) 771
- R. E. Schapire and Y. Freund, "Boosting: Foundations and Algorithms", MIT Press, 2012.
- Y. Freund and R.E. Schapire, "A decision-theoretic generalization of on-line learning and an application to boosting" ▸ Journal of Computer and System Sciences **55** (1997) 119
- J.H. Friedman, T. Hastie and R. Tibshirani, "Additive logistic regression: a statistical view of boosting" ▸ Annals of Statistics **28** (2000) 377

References II

- J. H. Friedman, "Greedy function approximation: A gradient boosting machine" ‣ Annals of Statistics **29** (2001) 1189
- T. Hastie, R. Tibshirani, and J. Friedman, "The Elements of Statistical Learning: Data Mining, Inference, and Prediction (2nd edition)" ‣ Springer Series in Statistics, 2009
- S. Shalev-Shwartz and S. Ben-David, "Understanding Machine Learning: From Theory to Algorithms" ‣ Cambridge University Press, 2014
- M. Belkin, D. Hsu, S. Ma, and S. Mandal, "Reconciling modern machine-learning practice and the classical bias–variance trade-off" ‣ PNAS **116** (2019) 15849, ‣ arXiv:1812.11118 [stat.ML]
- L. Breiman, "Bagging Predictors" ‣ Machine Learning **24** (1996) 123
- L. Breiman, "Random forests" ‣ Machine Learning **45** (2001) 5
- B. P. Roe, H.-J. Yang, J. Zhu, Y. Liu, I. Stancu, and G. McGregor ‣ Nucl. Instr. Meth. A **543** (2005) 577; H.-J. Yang, B.P. Roe, and J. Zhu ‣ Nucl. Instr. Meth. A **555** (2005) 370
- V. M. Abazov *et al.* [D0 Collaboration], "Evidence for production of single top quarks" ‣ Phys. Rev. D **78** (2008) 012005

Backup

- Pruning a decision tree
- ML training with TMVA

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

- *T*MVA: Toolkit for MultiVariate Analysis
  - https://root.cern/tmva
  - 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` -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,
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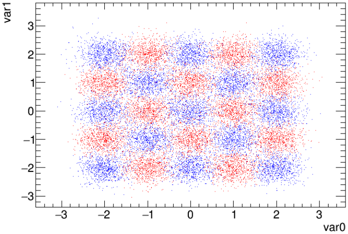
TFile* inputFile = new TFile("dataSchachbrett.root")
TTree* sig = (TTree*)inputFile->Get("TreeS");
TTree* bkg = (TTree*)inputFile->Get("TreeB");
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
```



Training with TMVA (Train.C)

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TMVA::DataLoader *dataloader =
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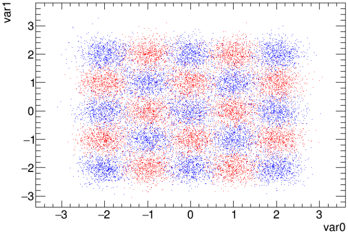
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
```



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dataloader->AddVariable("var0", 'F');
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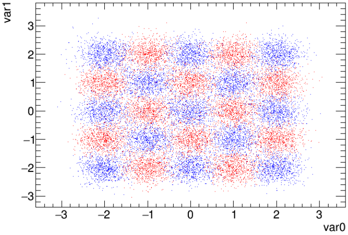
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
```



Training with TMVA (Train.C)

```
TFile* outputFile = TFile::Open("output.root","RECREATE");
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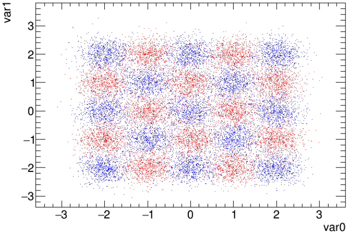
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!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");
```



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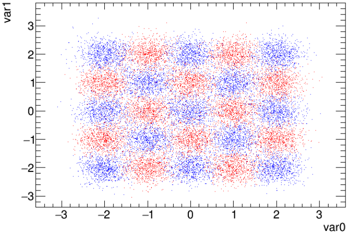
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
```



Training with TMVA (Train.C)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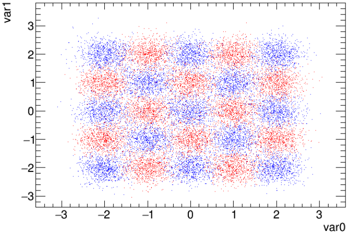
double sigWeight = 1.0; double bkgWeight = 1.0;
TMVA::DataLoader *dataloader =
    new TMVA::DataLoader("dataset");
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
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
```



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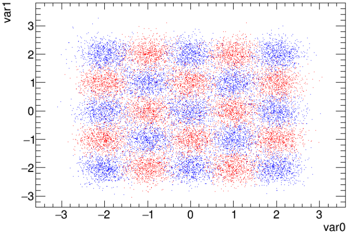
dataloader->AddVariable("var0", 'F');
dataloader->AddVariable("var1", 'F');
TCut mycut = "";
dataloader->PrepareTrainingAndTestTree(mycut,"SplitMode=Random");
factory->BookMethod(dataloader, TMVA::Types::kBDT, "BDT", "!H:!V:NTrees=400:
    MinNodeSize=4%:MaxDepth=5:BoostType=AdaBoost:AdaBoostBeta=0.15:nCuts=80");
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();
```



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TCut mycut = "";
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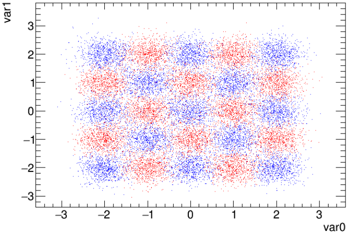
factory->TrainAllMethods(); // Train MVAs using training events
factory->TestAllMethods(); // Evaluate all MVAs using test events
// ----- Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
auto c1 = factory->GetROCCurve(dataloader); // Eager to compare performance
```



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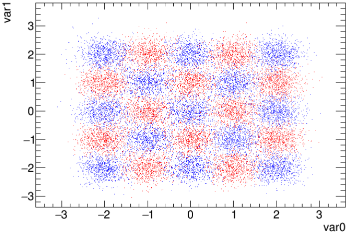
// ----- Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
auto c1 = factory->GetROCCurve(dataloader); // Eager to compare performance
outputFile->Close();
delete factory; delete dataloader;
```



Training with TMVA (Train.C)

```
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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:
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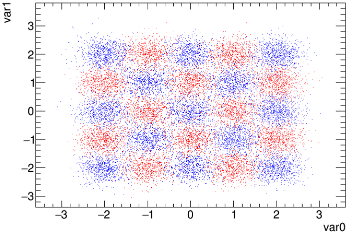
factory->BookMethod(dataloader, TMVA::Types::kFisher, "Fisher", "!H:!V:Fisher");
factory->TrainAllMethods(); // Train MVAs using training events
factory->TestAllMethods(); // Evaluate all MVAs using test events
// ----- Evaluate and compare performance of all configured MVAs
factory->EvaluateAllMethods();
auto c1 = factory->GetROCCurve(dataloader); // Eager to compare performance
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 );
```

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 );
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)

```
TFile* inputFile = new TFile("dataSchachbrett.root");
TTree* data = (TTree*)inputFile->Get("TreeS");
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");
// ------- 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");
Float_t var0=-99., var1=-99.;
data->SetBranchAddress("var0", &var0);
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reader->BookMVA( "My BDT", "dataset/weights/TMVAClassification_BDT.weights.xml");
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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();
```

- More complete tutorials:
  - https://github.com/lmoneta/tmva-tutorial

Compiling TMVA with C++

- To make code compilable (and MUCH faster)
  - Need ROOT and TMVA corresponding header files
  - e.g., for Train.C:

```
#include "TFile.h"
#include "TTree.h"
#include "TMVA/Factory.h"
#include "TMVA/DataLoader.h"
#include "TMVA/TMVAGui.h"
```

  - Need a “main” function

```
int main() {
  Train();
  return 0;
}
```

  - Compilation:

```
g++  Train.C ‘root-config --cflags --libs‘ -lTMVA  -lTMVAGui  -o  TMVATrainer
```

  - Train.C: file to compile
  - TMVATrainer: name of executable
  - -lTMVAGui: just because of `TMVA::TMVAGui("output.root");`

TMVA: training refinements

- Common technique: train on even event numbers, test on odd event numbers (and vice versa)
- Can also think of more than two-fold
- Achieve in TMVA by replacing:

```
dataloader->AddSignalTree(sig, sigWeight);
dataloader->AddBackgroundTree(bkg, bkgWeight);
```

- with:

```
TString trainString = "(eventNumber % 2 == 0)";
TString testString = "!"+trainString;
dataloader->AddTree(sig, "Signal", sigWeight, trainString.Data(), "Training");
dataloader->AddTree(sig, "Signal", sigWeight, testString.Data(), "Test");
dataloader->AddTree(bkg, "Background", bkgWeight, trainString.Data(), "Training");
dataloader->AddTree(bkg, "Background", bkgWeight, testString.Data(), "Test");
```

- Use individual event weights:

```
string eventWeight = "TMath::Abs(eventWeight)"; //Compute event weight
dataloader->SetSignalWeightExpression(eventWeight);
dataloader->SetBackgroundWeightExpression(eventWeight); //Can differ
```