Boosted decision trees

Yann Coadou

Centre de physique des particules de Marseille (CPPM), Aix Marseille Université, CNRS/IN2P3, Marseille, France
coadou@cppm.in2p3.fr

Boosted decision trees are a very powerful machine learning technique. After introducing specific concepts of machine learning in the high-energy physics context and describing ways to quantify the performance and training quality of classifiers, decision trees are described. Some of their shortcomings are then mitigated with ensemble learning, using boosting algorithms, in particular AdaBoost and gradient boosting. Examples from high-energy physics and software used are also presented.

To appear in Artificial Intelligence for High Energy Physics, P. Calafiura, D. Rousseau and K. Terao, eds. (World Scientific Publishing, 2022)
Contents

Boosted decision trees

1. Introduction .................................................. 3
2. Specificity of high-energy physics ............................ 3
2.1. Terminology ............................................... 4
2.2. Splitting samples for training ............................ 4
2.3. Cross-validation ........................................... 5
2.4. Using machine learning .................................... 6
2.5. Figures of merit ............................................ 6
2.5.1. ROC curve and area under the curve .................... 7
2.5.2. Significance ............................................. 8
2.6. Controlling overtraining .................................... 10
3. Decision trees .................................................. 12
3.1. Algorithm ................................................... 13
3.2. Tree hyperparameters ..................................... 16
3.3. Splitting a node ............................................ 17
3.4. Variable selection .......................................... 18
3.4.1. Manipulating variables .................................. 19
3.4.2. Mean decrease impurity ................................ 20
3.4.3. Permutation importance ................................. 20
3.4.4. Choosing variables ..................................... 21
3.5. Limitations .................................................. 22
3.5.1. Training sample composition ............................ 22
3.5.2. Pruning a tree .......................................... 22
3.5.3. Ensemble learning ....................................... 23
4. Boosted decision trees ......................................... 24
4.1. Introduction ................................................ 25
4.2. Boosting algorithm ........................................ 25
4.3. AdaBoost ................................................... 26
4.4. Gradient boosting ........................................... 30
4.5. Boosting examples ......................................... 31
4.5.1. The XOR problem ........................................ 32
4.5.2. Number of trees and overtraining ........................ 32
4.6. Other boosting algorithms ................................ 34
4.7. Boosted regression trees ................................... 36
4.8. Boosted decision trees in high-energy physics .......... 37
4.8.1. Use cases ............................................... 37
4.8.2. Systematic uncertainties ............................... 40
5. Other averaging techniques ................................... 41
6. Software ....................................................... 41
7. Conclusion ..................................................... 42
References ........................................................ 43
1. Introduction

Decision trees are a machine learning technique that appeared in the mid-1980’s and are still the subject of advanced studies in the field. Because it is a sophisticated supervised multivariate technique, learning from examples, it is important to remember that before applying it to real data (e.g. collisions from a high-energy physics experiment), it is crucial to have a good understanding of the data and of the physics model used to describe them (simulated samples, reconstruction and identification efficiencies, etc.). Any discrepancy between the real data and physics model (that is, features in the data that are not reproduced by the physics model because the simulation is incorrect or because the real data were not properly groomed) will provide an artificial separation that the decision trees will use, misleading the analyser. The hard (and interesting) part of the analysis is in building the proper physics model, not in ‘just’ extracting the signal. But once this is properly done, decision trees (and especially their boosted versions) provide a very powerful tool to increase the significance of any analysis.

Ever since their first use by the MiniBooNe collaboration for analysis and particle identification [1, 2] and by the D0 experiment for the first evidence of single top quark production [3, 4], boosted decision trees have been a primary tool in high energy physics to increase the discovery potential and measurement precision of experiments, in particular at the Tevatron and at the LHC. They are still highly relevant (and highly performing) in 2021, even though deep neural networks are becoming a serious contender.

As this is the first chapter of this book, some of the basic concepts useful in the context of high-energy physics when using most techniques presented in this and other chapters are summarised in Sec. 2. Section 3 explains how a decision tree is constructed, what parameters can influence its development and what its intrinsic limitations are. One possible extension of decision trees, boosting, is described in detail in Sec. 4, and other techniques trying to reach the same goal as boosting are presented in Sec. 5. Popular software implementations are introduced in Sec. 6, before reaching conclusions in Sec. 7.

2. Specificity of high-energy physics

All techniques presented in this book need to learn from examples. After a short list of definitions to have a common language between the physicist and the computer scientist in Sec. 2.1, several training strategies are
presented in Sec. 2.2, as well as how to deal with the samples to minimise training bias and maximise statistical power. In order to properly assess the performance of a classifier, cross-validation is introduced in Sec. 2.3. Section 2.4 describes typical usage of machine learning algorithms in high-energy physics. Several figures of merit are described in Sec. 2.5 and over-training is addressed in Sec. 2.6.

2.1. Terminology

Here are a few terms that take on different meanings in a high-energy physics or machine learning context.

**Event** All information collected during a collision inside a detector, or reproduced from a Monte Carlo simulation of such collisions (equivalent to a ‘sample’ in machine learning literature).

**Sample** A collection of events, a dataset.

**Variable** A property of the event or of one of its constituents (‘feature’ in machine learning)

**Cut** To cut on a variable is to apply a threshold on this variable and keep only events satisfying this condition. A cut-based analysis is applying such thresholds on several variables to select events.

**Event weight** In high-energy physics events usually have an associated weight, which depends on how many events were generated (relating to the process cross section and collected luminosity) and various corrections applied to simulations to account for differences between data and Monte Carlo predictions (jet energy scale or object identification efficiency are such weights). When using machine learning techniques all events are often treated equal by default. It is therefore important for the physicist to make sure to give the proper initial weight to all its input events. Then machine learning algorithms may internally reweight the events for their own purpose, but the starting point will correspond to the physical distributions. The concept is similar to importance weighting in machine learning, where events are given a larger weight to account, for instance, for their scarcity in the training sample.

2.2. Splitting samples for training

Decision trees, as many of the techniques presented in this book, belong to the class of algorithms using supervised learning: during training, the
classifier is presented only with events for which it knows features (discriminating variables) and class label (for instance in the binary case, whether the event is signal or background).

In order to not introduce bias, it is important to use an independent set of events during training, events that are then not used when performing a measurement. The usual approach is to split the dataset in three parts: a training sample from which to learn the task, a validation sample to evaluate performance and possibly optimise the classifier hyperparameters, and a testing sample for the actual measurement. In high-energy physics, simulated Monte Carlo events are often used for these three samples, and the performance on the testing sample is compared to that on data collected from the detector (never seen during training). Discrepancies between testing sample and data introduce a potential pitfall, that can be addressed with transfer learning and domain adaptation [5].

In general labelled data are ‘expensive’ to produce: hiring people to label images or translate speech, collecting X-ray images and medical diagnosis, etc. In high-energy physics very accurate, though not perfect, event generators and detector simulators are available. Models can be trained on the samples they provide, which are however quite costly in resources so that they should be used with parsimony. At the same time an increasing training set size is often associated with improved classifier performance. Monte Carlo samples can be split in half, one half for training (holding out part of this dataset for validation) and one for testing. By doing this half of the sample is ‘wasted’, not used for either training or testing, decreasing the quality of the training and of the measurement. The use of the sample can be maximised by performing two trainings: train the same classifier on the two halves (say, one on events with an even event number and one on events with an odd event number), and when testing, apply the classifier which did not see the event during training (so, the one trained on odd events is applied on even ones, and vice versa). The concept can be generalised to any number of splits, increasing the number of trained classifiers, each of them using a larger fraction of the available dataset for training.

2.3. Cross-validation

Training machine learning algorithms is usually a stochastic problem, the randomness coming from the training sample content, the optimisation process or the technique itself. This means that when training only once, there is a possibility to obtain an ‘abnormal’ result by chance, too good or too
bad compared to what could be expected. In high-energy physics some training samples may be limited in size and become very sensitive to this issue. To get a proper estimate of the mean performance and associated uncertainty (the variability of the algorithm output, originating from the training procedure), it may be better to perform several trainings. This principle was introduced with the so-called $K$-fold cross-validation, originally for decision trees [6]. After dividing a training sample $\mathcal{L}$ into $K$ subsets of equal size, $\mathcal{L} = \bigcup_{k=1..K} \mathcal{L}_k$, a classifier $T_k$ is trained on the $\mathcal{L} - \mathcal{L}_k$ sample and tested on $\mathcal{L}_k$. This produces $K$ classifiers, from which the mean performance and associated uncertainty is extracted. It helps in choosing the best model (each being tested with cross-validation), rather than relying on a single training for each model (which may or may not have an upward or downward performance fluctuation). Once the model is chosen, it can be retrained on the full (larger) training set, assuming its performance should approach the observed mean performance.

2.4. Using machine learning

This book describes various ways of using machine learning in high energy physics to accomplish many different tasks. Boosted decision trees are mostly used to separate a rare signal from a large background in physics analyses or to identify physics objects in the detector (see several use cases in Sec. 4.8.1). In practice these results are obtained in two ways. By applying a threshold on the boosted decision tree output a region or working point can be defined, as shown in Fig. 1(a): cutting at 0.83 defines a $b$-tagging working point with 70% efficiency on $b$-jets and a rejection factor (defined as the inverse of efficiency) of 313 (8) against light-flavoured jets (c-jets) [7]. The second approach consists in using the shape of the boosted decision tree output as the discriminating variable for the final analysis. As an example, in Fig. 1(b) the bins of ‘BDT score’ for all components of the physics model are included in a binned likelihood fit to the data. The low score values help constrain the background, and the high score bins reveal the need of the signal contribution to match the data, leading to the first evidence for the production of $t\bar{t}t\bar{t}$ in ATLAS [8].

2.5. Figures of merit

It is nowadays very easy, in just a few lines, to write the code to train and apply various machine learning algorithms, with several software options on the market (see Sec. 6). The lengthy part is more in the design and
optimisation of the model itself (that is, what algorithm, structure, hyperparameters to put in these few lines), and how to pick the best one. Several measures that are commonly used, in particular in high-energy physics, are presented below.

### 2.5.1. ROC curve and area under the curve

The receiver operating characteristic curve, or ROC curve, is a representation of the capacity of a binary classifier to separate the two classes, as its discrimination threshold is varied. It is plotting the true positive rate (or recall, a measure of the proportion of actual positives that are correctly identified as such) against the false positive rate (or fall-out, actual negatives improperly identified as positive), obtained when scanning the classifier output. In the context of signal and background, it shows signal efficiency versus background efficiency (or background rejection, defined as $1 - \text{efficiency}$). An example is shown in Fig. 2. In this convention, the better the classifier, the closer the curve is to the top right corner. The dashed line in the middle represents the performance of a classifier that is randomly guessing, rejecting or accepting 50% of signal and background in all cases. This is the worst achievable performance.

To compare ROC curves between classifiers, the area under the curve, AUC (hatched area in Fig. 2) can be computed. Perfect separation gives
Fig. 2. Example ROC curve. The hatched area is the area under the curve. The dashed line corresponds to random guessing.

an AUC of one, while random guessing corresponds to an AUC of 0.5.

A single number summary is of course practical, but hides details of the ROC curves being compared. If one ROC curve is systematically above the other, its AUC is larger and reflects better performance across the board. But if two ROC curves cross each other, then the interpretation of the AUC is more tricky: depending on the usage of the classifier, a higher curve at high background rejection may be more interesting than one at high efficiency for instance, so how to interpret the AUC is up to the analyser. To partially account for this effect it is also possible to compute the AUC only above a certain threshold.

2.5.2. **Significance**

In a physics analysis, the AUC is rarely the number of interest to optimise. It is more typical to aim for the best cross-section significance \( \frac{s}{\sqrt{s+b}} \) or excess significance \( \frac{s}{\sqrt{b}} \), where \( s \) (\( b \)) is the sum of weights (see Sec. 2.1) of signal (background) events. With \( n \) events in data, the observed significance is obtained by replacing \( s \) by \( n-b \). Given a machine learning algorithm output, typically in the range \([0, 1]\) or \([-1, 1]\), as is done when producing the ROC curve, \( s \) and \( b \) are computed above a threshold on the discriminant output, scanning its full range. It usually goes through a maximum towards high output values, before decreasing when statistics become too small. This maximum significance corresponds to the optimal value on which to cut on the discriminant to get the best possible analysis.

This simple-minded formula is very popular in high-energy physics but has shortcomings, and a refined version (counting experiment supposing a
single Poisson distributed value, with known background) gives the approximate median significance [9]:

\[ \text{AMS} = \sqrt{2 \left( (s + b) \ln \left( 1 + \frac{s}{b} \right) - s \right)} \]

Expanding the logarithm in \( s/b \) leads back to the previous formula, qualifying the validity of the approximation (requires \( s \ll b \)):

\[ \text{AMS} = \frac{s}{\sqrt{b}} (1 + O(s/b)) . \]

Optimising the AMS corresponds to optimising the ROC curve, focusing on the region with very high background rejection. This is the typical regime of a physics analysis.

There is usually an uncertainty on the background, which affects the significance. To extract their final results, modern analyses rely on advanced statistical models with a complex machinery (usually based on the RooStat framework [10]) accounting for all possible systematic effects. Running this whole infrastructure during machine learning training optimisation is usually prohibitive (complexity, CPU cost), so a simpler proxy to the analysis performance measure is necessary.

The simplest way to account partially for background uncertainty (\( \sigma_b \equiv ||b - b_{\text{sys}}|| \)) is to replace \( \sqrt{b} \) by the quadratic sum of \( \sqrt{b} \) and \( \sigma_b \):

\[ s \sqrt{b + \sigma_b^2} . \]

A refined version of the AMS can also take into account the background uncertainty [11]:

\[ \text{AMS}_1 = \sqrt{2 \left( (s + b) \ln \left( \frac{s + b}{b_0} \right) - (s - b + b_0) + \frac{(b - b_0)^2}{\sigma_b^2} \right)} , \]

with \( b_0 = \frac{1}{2} \left( b - \sigma_b^2 + \sqrt{(b - \sigma_b^2)^2 + 4(s + b)\sigma_b^2} \right) . \)

Expanding in powers of \( s/b \) and \( \sigma_b^2/b \) gives back the simpler formula:

\[ \frac{s}{\sqrt{b + \sigma_b^2}} \left( 1 + O(s/b) + O(\sigma_b^2/b) \right) . \]

Finally, to account for the shape of the discriminant rather than only choosing the best cut in a counting experiment, it is possible to replace
the global counts $s$, $b$ and $\sigma_b$ by their counts in each bin, summing up contributions of $N$ bins of discriminant output:

$$\text{AMS}_{i}^\text{sum} = \sqrt{\sum_{i}^{N} \left( 2 \left( (s_i + b_i) \ln \frac{s_i + b_i}{b_{0i}} - s_i - b_i + b_{0i} \right) + \frac{(b_i - b_{0i})^2}{\sigma_{bi}^2} \right)},$$

$$b_{0i} = \frac{1}{2} \left( b_i - \sigma_{bi}^2 + \sqrt{(b_i - \sigma_{bi}^2)^2 + 4(s_i + b_i)\sigma_{bi}^2} \right).$$

### 2.6. Controlling overtraining

Overtraining is what happens when a classifier learns too much about the specific details of the training sample, while these features are not representative of the underlying distributions. It may then be targeting noise, or misrepresent regions with too little statistics to train on. When applying such a classifier on the testing sample, its performance will be worse than that of a classifier immune to this issue, because it does not generalise well. It should be noted that what is often called overtraining here and in the following, in accordance with high-energy physics usage, is usually referred to as overfitting in the machine learning community. This is the so-called bias–variance trade-off [12]: it is difficult to minimise both the bias (the difference between the prediction of the model and the correct value it tries to predict) and variance (the variability of the model prediction for a given event, when considering multiple realisations of this same model). Increasing model complexity lowers the bias while increasing variance.

A particular type of overtraining is very easy to avoid, by following good practices from Sec. 2.2: never use training events when making the final measurement, which has to be performed on an independent set of events, never seen during training. Otherwise the performance will be artificially enhanced on the ‘testing’ sample and comparisons with the application to data will be impossible (or worse if not noticed).

Several techniques exist to mitigate overtraining, generically referred to as regularisation. They typically add a penalty for complexity to the loss function that is minimised during training (the function that maps each event to a real number quantifying the difference between the predicted and true classes or values). With classifier $f$ and loss function $L$, a regularisation term $R(f)$ is added to the loss function, which becomes $L(f) + \lambda R(f)$, where $\lambda$ is a parameter controlling the importance of the regularisation term. This will favour simpler models (increasingly simpler with larger values of $\lambda$, with the risk of underfitting with too much regularisation), less susceptible
to overtraining. $R(f)$ can take various forms, like L1 (L2) regularisation based on the sum of weights (sum of squared weights) used to describe neural networks, or the number and depth of trees (see Sec. 3.5.2). Sparsity (setting many weights to zero [13]) and dropout (randomly dropping out nodes during training [14]) are more recent very effective approaches for neural networks. Ensemble learning (see Sec. 3.5.3 and Sec. 5) is another approach.

It is important to check whether the model suffers from overtraining. As shown in Fig. 3 this can be achieved by monitoring the error rate (or the loss function) during training, as a function of the number of trees with boosted decision trees or training epoch with neural networks, on the training and validation samples. Figure 3(a) is the canonical example of such curves. The training error tends towards zero, while the testing curve first follows the training curve, reaches a minimum and increases again. The best classifier is the one at the minimum, training further will reduce performance and cause overfitting: the classifier has too much capacity (complexity) with respect to the training sample. Selecting the model at the minimum means early stopping [12].

In many cases though, the situation is similar to Fig. 3(b): the training and testing curves follow each other but start diverging while still both improving. The classifier is therefore already learning specificities of the training set, but still learning properties that generalise well and improve performance on the validation set. The testing curve goes through a minimum, corresponding to the best model, and increases again, this time showing detrimental overtraining as the performance decreases on the validation set (overfitting regime). This is the typical U-shaped curve arising from the bias–variance trade-off.

The curves could also look like Fig. 3(c), where the testing curve never goes through a minimum and instead flattens. Once in the plateau, all classifiers are equivalent in terms of performance on the validation set, while the training error keeps improving (and could reach zero, this is the so-called interpolation regime [15])). This is a typical curve for boosted decision trees.

Finally the situation could correspond to Fig. 3(d). At the interpolation threshold the training error reaches zero, but continued training of high capacity classifiers leads to a double descent curve: the testing performance keeps increasing while the training error stays at zero [16].
Fig. 3. Overtraining estimation using the error rate as a function of the number of trees (for boosted decision trees) or epochs (for neural networks). Black curves are measured on the training sample and red curves on the validation sample. The optimal classifier corresponds to the ‘best’ label. The hatched areas represent overtraining: beneficial in blue (but underfitting), detrimental in orange (overfitting). (a) Typical curves, with the best model at the minimum of the testing curve, and overfitting beyond with decrease of performance. (b) The best model is overtrained but still improves performance. (c) Typical curves for boosted decision trees with flattening testing error rate: all models in the flat area perform equally well despite increasing overtraining. (d) Interpolation regime: the best classifier is obtained after the training error has reached zero.

3. Decision trees

Decision trees are a machine learning technique first developed in the context of data mining and pattern recognition [6], which then gained momentum in various fields, including medical diagnosis [17, 18], insurance and loan screening, or optical character recognition of handwritten text [6].

It was developed and formalised by Breiman et al. [6] who proposed the CART algorithm (Classification And Regression Trees) with a complete
and functional implementation of decision trees.

The basic principle is rather simple: it consists in extending a simple cut-based analysis into a multivariate technique by continuing to analyse events that fail a particular criterion. Many, if not most, events do not have all characteristics of either signal or background (for a two-class problem). The concept of a decision tree is therefore to not reject right away events that fail a criterion, and instead to check whether other criteria may help to classify these events properly.

In principle a decision tree can deal with multiple output classes, each branch splitting in many subbranches. In this chapter almost only binary trees will be considered, with only two possible classes: signal and background. The same concepts generalise to non-binary trees, possibly with multiple outputs.

Section 3.1 describes the decision tree building algorithm, controlled by hyperparameters presented in Sec. 3.2. The way to split nodes is explained in Sec. 3.3, while Sec. 3.4 describes how decision trees can advantageously deal with input variables and how to optimise their list. Finally Sec. 3.5 reports several shortcomings of decision trees, with suggestions to address them.

3.1. Algorithm

Mathematically, decision trees are rooted binary trees (as only trees with two classes, signal and background, are considered). An example is shown in Fig. 4. A decision tree starts from an initial node, the root node. Each node can be recursively split into two daughters or branches, until some stopping condition is reached. The different aspects of the process leading to a full tree, indifferently referred to as growing, training, building or learning, are described in the following sections.

Consider a sample of signal ($s_i$) and background ($b_j$) events, each with weights $w_{s_i}$ and $w_{b_j}$, respectively, described by a set $\vec{x}_i$ of variables. This sample constitutes the root node of a new decision tree.

Starting from this root node, the algorithm proceeds as follows:

1. If the node satisfies any stopping criterion, declare it as terminal (that is, a leaf) and exit the algorithm.
2. Sort all events according to each variable in $\vec{x}$.
3. For each variable, find the splitting value that gives the best separation between two children, one with mostly signal events, the other with mostly background events (see Sec. 3.3 for details). If the separation
cannot be improved by any splitting, turn the node into a leaf and exit the algorithm.

(4) Select the variable and splitting value leading to the best separation and split the node in two new nodes (branches), one containing events that fail the criterion and one with events that satisfy it.

(5) Apply recursively from step 1 on each node.

This is a greedy algorithm, not guaranteed to find the optimal solution. At each node, all variables can be considered, even if they have been used in a previous iteration: this allows to find intervals of interest in a particular variable, instead of limiting oneself to using each variable only once.

It should be noted that a decision tree is human readable: exactly which criteria an event satisfied in order to reach a particular leaf can be traced. It is therefore possible to interpret a tree in terms of, e.g., physics, defining selection rules, rather than only as a mathematical object.

In order to make the whole procedure clearer, let us take the tree in Fig. 4 as an example. Consider that all events are described by three variables: $x$, $y$ and $z$. All signal and background events make up the root node.

![Graphical representation of a decision tree](image)

**Fig. 4.** Graphical representation of a decision tree. Blue rectangles are internal nodes with their associated splitting criterion; leaves are terminal nodes with their purity.
All events are first sorted according to each variable:
\[ x^{s_1} \leq x^{b_3} \leq \ldots \leq x^{b_2} \leq x^{s_{12}}, \]
\[ y^{b_5} \leq y^{b_3} \leq \ldots \leq y^{s_{67}} \leq y^{s_{43}}, \]
\[ z^{b_6} \leq z^{s_8} \leq \ldots \leq z^{s_{12}} \leq z^{b_9}, \]
where superscript \( s_i \) (\( b_j \)) represents signal (background) event \( i \) (\( j \)). Using some measure of separation between classes (see below) the best splitting for each variable may be (arbitrary unit):
\[ x < 1.53 \text{ separation } = 5, \]
\[ y < 0.01 \text{ separation } = 3, \]
\[ z < 25 \text{ separation } = 0.7. \]

The best split is \( x < 1.53 \), and two new nodes are created, the left one with events failing this criterion and the right one with events satisfying it. The same algorithm is applied recursively to each of these new nodes. As an example consider the right-hand-side node with events that satisfied \( x < 1.53 \). After sorting again all events in this node according to each of the three variables, it was found that the best criterion was \( x < 1.8 \), and events were split accordingly into two new nodes. This time the right-hand-side node satisfied one of the stopping conditions and was turned into a leaf. From signal and background training events in this leaf, the purity was computed as \( p = 0.91 \). The left-hand-side node keeps splitting further.

The decision tree output for a particular event \( i \) is defined by how its \( \vec{x}_i \) variables behave in the tree:

1. Starting from the root node, apply the first criterion on \( \vec{x}_i \).
2. Move to the passing or failing branch depending on the result of the test.
3. Apply the test associated to this node and move left or right in the tree depending on the result of the test.
4. Repeat step 3 until the event ends up in a leaf.
5. The decision tree output for event \( i \) is the value associated with this leaf.

There are several conventions used for the value attached to a leaf. It can be the purity \( p = \frac{s}{s+b} \) where \( s \) (\( b \)) is the sum of weights of signal (background) events that ended up in this leaf during training. It is then bound to \([0,1]\), close to 1 for signal and close to 0 for background.

It can also be a binary answer, signal or background (mathematically typically +1 for signal and 0 or −1 for background) depending on whether
the purity is above or below a specified critical value (e.g. \( +1 \) if \( p > \frac{1}{2} \) and \(-1\) otherwise).

Looking again at the tree in Fig. 4, the leaf with purity \( p = 0.91 \) would give an output of 0.91, or +1 as signal if choosing a binary answer with a critical purity of 0.5.

### 3.2. Tree hyperparameters

The number of hyperparameters of a decision tree is relatively limited. The first one is not specific to decision trees and applies to most techniques requiring training: how to normalise signal and background with respect to each other before starting the training? Conventionally the sums of weights of signal and background events are chosen to be equal (balanced classes), giving the root node a purity of 0.5, that is, an equal mix of signal and background. Decision trees are not particularly sensitive to this original normalisation as in practice, a few early splits will produce nodes with more balanced categories, therefore only leading to a limited inefficiency in the training process which only impacts marginally the final discriminating power.

Other hyperparameters concern the selection of splits. A list of discriminating variables is needed, and a way to evaluate the best separation between signal and background events (the goodness of the split). Both aspects are described in more detail in Sec. 3.3 and Sec. 3.4.

The splitting has to stop at some point, declaring such nodes as terminal leaves. Conditions to satisfy can include:

- a minimum leaf size. A simple way is to require at least \( N_{\text{min}} \) training events in each node after splitting, to ensure the statistical significance of the purity measurement, with a statistical uncertainty \( \sqrt{N_{\text{min}}} \). It becomes a little bit more complicated with weighted events, as is normally the case in high-energy physics applications. Using the effective number of events instead may be considered:

  \[
  N_{\text{eff}} = \frac{\left( \sum_{i=1}^{N} w_i \right)^2}{\sum_{i=1}^{N} w_i^2},
  \]

  for a node with \( N \) events associated to weights \( w_i \) (\( N_{\text{eff}} = N \) for unweighted events).

- having reached perfect separation (all events in the node belong to the same class).

- an insufficient improvement with further splitting.
• a maximum tree depth, if the tree cannot have more than a certain number of layers (for purely computational reasons or to have like-size trees).

Finally a terminal leaf has to be assigned to a class. This is classically done by labelling the leaf as signal if \( p > 0.5 \) and background otherwise.

### 3.3. Splitting a node

The core of a decision tree algorithm resides in how a node is split into two. Consider an impurity measure \( i(t) \) for node \( t \), which describes to what extent the node is a mix of signal and background. Desirable features of such a function are that it should be:

- maximal for an equal mix of signal and background (no separation).
- minimal for nodes with either only signal or only background events (perfect separation).
- symmetric in signal and background purities, as isolating background is as valuable as isolating signal.
- strictly concave in order to reward purer nodes. This tends to favour asymmetric end cuts with one smaller node and one larger node.

A figure of merit can be constructed with this impurity function, as the decrease of impurity for a split \( S \) of node \( t \) into two children \( t_P \) (pass) and \( t_F \) (fail):

\[
\Delta i(S, t) = i(t) - p_P \cdot i(t_P) - p_F \cdot i(t_F),
\]

where \( p_P \) (\( p_F \)) is the fraction of events that passed (failed) split \( S \).

The goal is to find the split \( S^* \) that maximises the decrease of impurity:

\[
\Delta i(S^*, t) = \max_{S \in \{\text{splits}\}} \Delta i(S, t).
\]

It will result in the smallest residual impurity, which minimises the overall tree impurity.

A stopping condition can be defined using the decrease of impurity, not splitting a node if \( \Delta i(S^*, t) \) is less than some predefined value. Such early-stopping criterion requires care, as sometimes a seemingly very weak split may allow child nodes to be powerfully split further (see Sec. 3.5.2 about pruning).

Common impurity functions (exhibiting most of the desired features mentioned previously) are illustrated in Fig. 5:
• the misclassification error: \(1 - \max(p, 1 - p)\),

• the (cross) entropy [6]: \(-\sum_{i=s,b} p_i \log p_i\), with \(p_b = 1 - p_s\) and \(p_s = p\),

• the Gini index of diversity [19].

The Gini index is the most popular in decision tree implementations. It typically leads to similar performance to entropy.

![Impurity measures as a function of signal purity.](image)

Other measures are also used sometimes, which do not satisfy all criteria listed previously but attempt at optimising signal significance, a typical final goal in high-energy physics applications (see Sec. 2.5.2):

• cross section significance (optimising \(\frac{s}{\sqrt{s + b}}\)): \(-\frac{s^2}{s + b}\),

• excess significance (optimising \(\frac{s}{\sqrt{b}}\)): \(-\frac{s^2}{b}\).

### 3.4. Variable selection

Overall decision trees are very resilient to most factors affecting variables. They are not too much affected by the ‘curse of dimensionality’, which forbids the use of too many variables in most multivariate techniques. For decision trees the CPU consumption scales as \(nN\log N\) with \(n\) variables and \(N\) training events. It is not uncommon to encounter decision trees using tens [4] or hundreds [2] of variables, although this is usually frowned upon in high-energy physics: more variables means more distributions and correlations to check, more complex interplay with systematic uncertainties, more dependence on the Monte Carlo event properties that are usually used during training and may not match real data so well, so physicists tend to reduce the list of discriminating variables to typically 10–15. On the other hand adding variables tends to always improve the performance of decision trees (see Sec. 4.8.1 for an example).
3.4.1. Manipulating variables

With most machine learning algorithms, a careful preparation of inputs is necessary to achieve good performance. Although not detrimental to decision trees, such manipulations are not really compulsory as decision trees tend to be very stable under such transforms.

A decision tree is immune to duplicate variables: the sorting of events according to each of them would be identical, leading to the exact same tree. The order in which variables are presented is completely irrelevant: all variables are treated equal. The order of events in the training samples is also irrelevant.

If variables are not very discriminating, they will simply be ignored and will not add any noise to the decision tree. The final performance will not be affected, it will only come with some CPU overhead during both training and evaluation.

Decision trees can deal easily with both continuous and discrete variables, simultaneously.

Another typical task before training a multivariate technique is to transform input variables by for instance making them fit in the same range (normalisation), having unit variance (standardisation) or taking the logarithm to regularise the variable. This is totally unnecessary with decision trees, which are completely insensitive to the replacement of any subset of input variables by (possibly different) arbitrary strictly monotone functions of them (e.g. converting MeV to GeV), as the same ordering of events would induce the same splits on the dataset, producing the same decision tree. This means that decision trees have some immunity against outliers. The above is strictly true only if testing all possible cut values while evaluating the optimal split. If there is some computational optimisation (e.g., check only 20 possible cuts on each variable), it may not work anymore and some transformation of inputs may be beneficial, at the very least to speed up convergence (numerical precision could also be a factor).

If linear correlations exist between variables, first decorrelating the input variables and then feeding them to the decision tree may help. If not doing this decorrelation, a decision tree will anyway find the correlations but in a very suboptimal way, by successive approximations, adding complexity to the tree structure without performance gain.
3.4.2. Mean decrease impurity

It is possible to rank variables in a decision tree, adding up the decrease of impurity (see Sec. 3.3) for each node where the variable was used to split, hence computing the mean decrease impurity (MDI). The variable with the largest decrease of impurity is the best variable. A shortcoming of this approach is that it is computed on the training set only, and may be exaggerating the importance of some variables because of overfitting.

There is another shortcoming with variable ranking in a decision tree: variable masking. Variable $x_j$ may be just a little worse than variable $x_i$ and would end up never being picked in the decision tree growing process. Variable $x_j$ would then be ranked as irrelevant. But if $x_i$ were removed, then $x_j$ would become very relevant. Note that this is not important in terms of pure performance of the tree: it did find the optimal way to use both variables in this particular training. If trying to learn something from the tree structure on the other hand, like deriving selection rules, this phenomenon will interfere with the potential understanding.

There is a solution to this feature, called surrogate splits [6]. For each split, a comparison is made between training events that pass or fail the optimal split and events that pass or fail a split on another variable. The split that mimics best the optimal split is called the surrogate split. This can be taken into consideration when ranking variables. It has applications in case of missing data: the optimal split can be replaced by the surrogate split.

All in all, variable rankings should never be taken at face value. They do provide valuable information but should not be over-interpreted.

3.4.3. Permutation importance

The shortcomings of MDI discussed above are partially addressed with a different technique called permutation importance or mean decrease accuracy (MDA). While MDI mostly works for decision trees, permutation importance is suited for all models using tabular data. It is defined as the decrease of performance of an already trained model when applying it on a sample after randomly shuffling a single discriminating variable [20]. If the variable is of any use, the performance should decrease when submitted to this noisy input, and more so if the tree relies heavily on this feature for its prediction. Repeating this for all input variables, the importance of each of them can be ranked. The operation can be done multiple times, shuffling each variable differently, in order to get a mean value and uncertainty on
variable importance. As with MDI, the measured importance is not telling anything about the intrinsic merit of a single variable (in terms of physics meaning for instance), but is rather a measure of its importance for this particular training.

Another advantage of this approach is that it can be applied on the validation set as well. Variables that are important on the training set but not on the validation set may be a source of overfitting.

As with MDI however, correlations may hide the intrinsic performance of a variable. If two variables are correlated and only one is shuffled, the proper information is still accessible, giving a lower importance to both. Once again, interpreting variable rankings must be done with care.

3.4.4. Choosing variables

It may sound obvious that only well discriminating variables should be used as input features to the decision tree training. It is nevertheless not trivial to achieve: variables are often correlated, they come in large numbers, and can be more or less discriminating in various regions of the input-feature phase space. The decision tree will isolate sub-regions, whose properties are not readily available when measuring any kind of discrimination in the full training set.

Brute force is a possibility: with a limited number of $N$ features, train all possible combinations of $N$, $N - 1$, etc., variables, and pick the best one according to some metric (see Sec. 2.5). In reality this becomes quickly impractical.

Instead, a commonly used approach in high-energy physics is backward elimination [21], which starts from the full list of $N$ variables used to train a tree ($T_N$). Then train all decision trees with $N - 1$ variables and keep the best performing one on the validation set ($T_{N-1}$). Starting from these $N - 1$ variables, train all decision trees with $N - 2$ variables to build $T_{N-2}$, and so on. Usually the performance of tree $T_k$ will decrease with $k$, and it is up to the analyser to decide how much performance to lose compared to getting a simpler (possibly more robust) tree. This is the usual trade-off of cost and complexity.

The selection can also be done in reverse, starting from $k = 1$ variable, training all trees with $k + 1$ variables, keeping the best one on the validation set and moving to $k + 2$ variables, until $k = N$ (forward greedy selection [21]). The advantage is that one can stop adding variables once the performance curve seems to saturate. It is on the other hand not equivalent
to backward elimination, as it may miss powerful variable combinations.

It can be tempting to train a tree with many variables and then remove the lowest ranked. Although quicker, it will most certainly be suboptimal because of the shortcomings of such rankings, as described in Sec. 3.4.2 and Sec. 3.4.3. The ranking is only relevant to the corresponding tree, and as soon as one of the variables is removed the others may be reshuffled.

3.5. Limitations

Despite all the nice features presented above, decision trees are known to be relatively unstable. If trees are too optimised for the training sample, they may not generalise very well to unknown events, as they would depend on the training sample (see Sec. 3.5.1). This can be mitigated with pruning, described in Sec. 3.5.2. Combining several classifiers can also improve the overall performance, as shown in Sec. 3.5.3.

3.5.1. Training sample composition

A small change in the training sample can lead to drastically different tree structures (high variance), rendering the physics interpretation a bit less straightforward. As such, a decision tree is not stable, where stability means that a slight change of the inputs does not change much the output [21]. For sufficiently large training samples, the performance of these different trees will be equivalent, but on small training samples variations can be very large. This does not give too much confidence in the result.

Moreover a decision tree output is by nature discrete, limited by the purities of all leaves in the tree. To decrease the discontinuities the tree size and complexity has to increase, which may not be desirable or even possible. Then the tendency is to have spikes in the output distribution at specific purity values, or even two delta functions at $\pm 1$ if using a binary answer rather than the purity output.

3.5.2. Pruning a tree

When growing a tree, each node contains fewer and fewer events, leading to an increase of the statistical uncertainty on each new split. The tree will tend to become more and more specialised, focusing on properties of the training sample that may not reflect the expected result, had there been infinite statistics to train on. Its variance increases.
A first approach to mitigate this effect and keep the variance under control, sometimes referred to as pre-pruning, has already been described in Sec. 3, using stopping conditions. The limitation is that requiring too big a minimum leaf size or too much of an improvement may prevent further splitting that could be very beneficial later on.

Another approach consists in building a very large tree and then cutting irrelevant branches (which target too closely the training sample and would not generalise well) by turning an internal node and all its descendants into a leaf, removing the corresponding subtree. This is post-pruning, or simply pruning.

There are many different pruning algorithms available. Expected error pruning [22] starts from a fully grown tree and compares the expected error of a node to the weighted sum of expected errors from its children. If the expected error of the node is less than that of the children, then the node is pruned. This does not require a separate pruning sample. With reduced error pruning [22] the misclassification rate on a pruning sample for the full tree is compared to the misclassification rate when a node is turned into a leaf. If the simplified tree has better performance, the subtree is pruned. Finally cost–complexity pruning is part of the CART algorithm [6] and the most used. Starting from a fully grown tree, the cost–complexity is computed as the sum of misclassification rate and a term proportional to the number of nodes in the tree (the complexity part, penalising larger trees). A sequence of decreasing cost–complexity subtrees is generated, and their misclassification rate on the pruning sample is computed. It will first decrease, and then go through a minimum before increasing again. The optimally pruned tree is the one corresponding to the minimum.

It should be noted that the best pruned tree may not be optimal or necessary when part of a forest of trees, such as those introduced in the next Sections.

3.5.3. Ensemble learning

Pruning is helpful in maximising the generalisation potential of a single decision tree. It nevertheless does not address other shortcomings of trees like the discrete output or lack of stability. A way out is to proceed with averaging several trees, with the added potential bonus that the discriminating power may increase. Such approaches belong to the general theoretical framework of ensemble learning [23]. Many averaging techniques have been developed. Bagging, boosting and random forests are such techniques and
will be described in the following Sections.

The power of ensemble learning resides in the much richer description of the input patterns when using several classifiers simultaneously. It is applicable to other machine learning techniques than decision trees. As shown in the example of Fig. 6(a) in a simple 2D case, a classifier may split the space in two (partitions 1/2/3), but three classifiers each doing this can possibly give more complete information about seven regions, each region being represented by three numbers (C1/C2/C3). When all three classifiers give the same answer, the confidence increases. Using decision trees as in Fig. 6(b), three simple decision trees give a crude separation of classes 1 and 2, while averaging them produces a decision contour that is much closer to the actual class separation.

![Fig. 6.](a) Description of 2D space combining three discriminants. (b) Three separate decision trees and their combination [24].

4. Boosted decision trees

As will be shown in this section, the boosting algorithm has turned into a very successful way of improving the performance of any type of classifier, not only decision trees. After a short history of boosting in Sec. 4.1, the generic algorithm is presented in Sec. 4.2 and specific implementations (AdaBoost and gradient boosting) are described in Secs. 4.3 and 4.4. Boosting is illustrated with a few examples in Sec. 4.5. Other boosting implementations are shown in Sec. 4.6. The use of boosting for regression rather than classification is presented in Sec. 4.7. Finally the application of boosted decision trees in high-energy physics, where it is so far the machine learning algorithm of choice, is illustrated in Sec. 4.8.
4.1. Introduction

The first provable algorithm of boosting was proposed in 1990 [25]. It worked in the following way:

- train a classifier $T_1$ on a sample of $N$ events;
- train $T_2$ on a new sample with $N$ events, half of which were misclassified by $T_1$;
- build $T_3$ on events where $T_1$ and $T_2$ disagree.

The boosted classifier was defined as a majority vote on the outputs of $T_1$, $T_2$ and $T_3$.

Following up on this idea boosting by majority [26] was introduced in 1995. It consisted in combining many learners with a fixed error rate. This was an impractical prerequisite for a viable automated algorithm, but was a stepping stone to the first functional boosting algorithm, called AdaBoost [27].

Boosting, and in particular boosted decision trees, have become increasingly popular in high-energy physics and are extensively used in physics analyses and object identification at the Tevatron and the LHC (see Sec. 4.8 for a few examples).

4.2. Boosting algorithm

It is hard to make a very good discriminant, but relatively easy to make simple ones which are certainly more error-prone (high bias) but are still performing at least marginally better than random guessing. Such discriminants are called weak classifiers. The goal of boosting is to combine such weak classifiers into a new, more stable one, with a smaller error rate (with lower bias than the individual classifiers) and better performance.

Consider a training sample $T_k$ containing $N_k$ events. The $i$th event is associated with a weight $w_k^i$, a vector of discriminating variables $\vec{x}_i$ and a class label $y_i = +1$ for signal, $-1$ for background. The pseudocode for a generic boosting algorithm is:

Initialise $T_1$
for $k$ in 1..$N_{\text{tree}}$
  train classifier $T_k$ on $T_k$
  assign weight $\alpha_k$ to $T_k$
  modify $T_k$ into $T_{k+1}$

The boosted output is some function $F(T_1, ..., T_{N_{\text{tree}}})$, typically a
weighted average:

\[ F(i) = \sum_{k=1}^{N_{\text{tree}}} \alpha_k T_k(\vec{x}_i). \]

Thanks to this averaging, the output becomes quasi-continuous, mitigating one of the limitations of single decision trees (see Sec. 3.5.1).

Note that in this process, once a particular tree is trained it is never modified, but just added to the mix. This is a different approach from, e.g., neural networks, in which the same weights are repeatedly updated over epochs to converge towards the final classifier.

4.3. AdaBoost

One particularly successful implementation of the boosting algorithm is AdaBoost [27]. AdaBoost stands for adaptive boosting, referring to the fact that the learning procedure adjusts itself to the training data in order to classify it better. There are many variations for the actual implementation, and it is the most common boosting algorithm. It typically leads to better results than without boosting, up to the Bayes limit as will be seen later.

An actual implementation of the AdaBoost algorithm works as follows. After having built tree \( T_k \), events in the training sample \( T_k \) that are misclassified by \( T_k \) should be checked, hence defining the misclassification rate \( R(T_k) \). In order to ease the math, let us introduce some notations. Define \( I: X \to \{0,1\} \) such that \( I(X) = 1 \) if statement \( X \) is true, and 0 otherwise. A function can now be defined that tells whether an event is misclassified by \( T_k \). In the decision tree output convention of returning only \{±1\} it gives:

\[ \text{isMisclassified}_k(i) = I(y_i \times T_k(i) \leq 0), \]

while in the purity output convention (with a critical purity of 0.5) it leads to:

\[ \text{isMisclassified}_k(i) = I(y_i \times (T_k(i) - 0.5) \leq 0). \]

The misclassification rate is now:

\[ R(T_k) = \varepsilon_k = \frac{\sum_{i=1}^{N_k} w^k_i \times \text{isMisclassified}_k(i)}{\sum_{i=1}^{N_k} w^k_i}. \]

This misclassification rate can be used to derive a weight associated to tree \( T_k \):

\[ \alpha_k = \beta \times \ln \frac{1 - \varepsilon_k}{\varepsilon_k}, \]
where $\beta$ is a free parameter to adjust the strength of boosting (set to one in the original algorithm). Similarly to the naming convention of other machine learning algorithms, it can be seen as a learning rate or shrinkage coefficient and drives how aggressive boosting should be.

The core of the AdaBoost algorithm resides in the following step: each event in $T_k$ has its weight changed in order to create a new sample $T_{k+1}$ such that:

$$w^k_i \rightarrow w^{k+1}_i = w^k_i \times e^{\alpha_k \cdot \text{isMisclassified}_k(i)}.$$ 

This means that properly classified events are unchanged from $T_k$ to $T_{k+1}$, while misclassified events see their weight increased by a factor $e^{\alpha_k}$. The next tree $T_{k+1}$ is then trained on the $T_{k+1}$ sample. This next tree will therefore see a different sample composition with more weight on previously misclassified events, and will therefore try harder to classify properly difficult events that tree $T_k$ failed to identify correctly, while leaving alone those events that previous iterations can handle properly. The final AdaBoost result for event $i$ is:

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

As an example, assume for simplicity the case $\beta = 1$. A not-so-good classifier, with a misclassification rate $\varepsilon = 40\%$ would have a corresponding $\alpha = \ln \frac{0.6}{0.4} = 0.4$. All misclassified events would therefore get their weight multiplied by $e^{0.4} = 1.5$, and the next tree will have to work a bit harder on these events. Now consider a good classifier with an error rate $\varepsilon = 5\%$ and $\alpha = \ln \frac{0.95}{0.05} = 2.9$. Misclassified events get a boost of $e^{2.9} = 19$ and will contribute decisively to the structure of the next tree! This shows that being failed by a good classifier brings a big penalty.

It can be shown [28] that the misclassification rate $\varepsilon$ of the boosted result on the training sample is bounded from above:

$$\varepsilon \leq \prod_{k=1}^{N_{\text{tree}}} 2\sqrt{\varepsilon_k (1 - \varepsilon_k)}.$$ 

If each tree has $\varepsilon_k \neq 0.5$, that is to say, if it does better than random guessing, then the conclusion is quite remarkable: the error rate falls to zero for a sufficiently large $N_{\text{tree}}$. A corollary is that the training data is overfit.

Overtraining is usually regarded as a negative feature. Does this mean that boosted decision trees are doomed because they are too powerful on the
training sample? Not really. As shown in Sec. 2.6 what matters most is not the error rate on the training sample, but rather the error rate on the testing sample. In the case of Fig. 3(a) or Fig. 3(b) boosting should stop when the minimum is reached (early stopping). It has however been routinely observed [29–31] that boosted decision trees often do not go through such a minimum, but rather tend towards a plateau in testing error (see Fig. 3(c)). Boosting could be stopped after having reached this plateau.

In a typical high-energy physics problem, the error rate may not even be what should be optimised. A good figure of merit on the testing sample would rather be the significance. Figure 7(a) illustrates this behaviour, showing how the significance saturates with an increasing number of boosting cycles. Arguably one could stop before the end and save resources, but at least the performance does not deteriorate with increasing boosting.

![Graphs](https://example.com/fig7.png)

**Fig. 7.** Behaviour of boosting. (a) Significance as a function of the number of boosted trees. (b) Signal efficiency vs. background efficiency for single and boosted decision trees, on the training and testing samples. (c) Misclassification rate of each tree as a function of the number of boosted trees. (d) Weight of each tree as a function of the number of boosted trees.
Another typical curve to optimise is the signal efficiency vs. the background efficiency (the ROC curve, see Sec. 2.5.1). Figure 7(b) clearly exemplifies this interesting property of boosted decision trees. The performance is clearly better on the training sample than on the testing sample (the training curves are getting very close to the upper left corner of perfect separation), with a single tree or with boosting, a clear sign of overtraining. But the boosted tree is still performing better than the single tree on the testing sample, proof that it does learn something more than memorising the training sample.

No clear explanation has emerged as to why boosting leads to such features, with typically no loss of generalisation performance due to overtraining, but some ideas have come up. It may have to do with the fact that during the boosting sequence, the first tree is the best while the others are successive minor corrections, which are given smaller weights. This is shown in Fig. 7(c) and Fig. 7(d), where the misclassification rate of each new tree separately is actually increasing, while the corresponding tree weight is decreasing. This is not surprising: during boosting the successive trees are specialising on specific event categories, and can therefore not perform as well on other events. So the trees that lead to a perfect fit of the training data are contributing very little to the final boosted decision tree output on the testing sample. When boosting decision trees, the last tree is not an evolution of the first one that performs better, quite the contrary. The first tree is typically the best, while others bring dedicated help for misclassified events. The power of boosting does not rely in the last tree in the sequence, but rather in combining a suite of trees that focus on different events.

A probabilistic interpretation of AdaBoost was proposed [31] which gives some insight into the performance of boosted decision trees. It can be shown that for a boosted output $T$ flexible enough:

$$e^{T(i)} = \frac{p(S|i)}{p(B|i)}$$

This means that the AdaBoost algorithm will tend towards the Bayes classifier, the maximum reachable separation.

Finally AdaBoost performance and its tendency to generalise well despite matching very closely the training data (to the extent that in many documented cases, to keep boosting even after the training error has reached zero still improves the performance on the testing sample [29], in the interpolation regime [15]) have been qualitatively understood with the margins explanation [29, 32]. A classifier can be more sure of some predictions than
of others (recall Fig. 6(a)), and could then generalise better. By boosting, AdaBoost tends to increase the margins on the training set, even after reaching zero training error. For each event, the margin accounts for the separability between classes, measured by the proportion of trees that misclassify each event. For event $x$ with truth label $y$ the margin $y \times T(x)$ for boosted decision tree $T$ is:

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

that is, the difference between the weights of single trees that classify $x$ correctly and the weights of trees that misclassify $x$. Boosting more means adding small corrections that tend to increase the margin for each event. This increases the confidence in the prediction, more likely to be correct. It makes a link with support vector machines [33], although this did not bring great insights to improve AdaBoost in the end.

This shortcoming suggests that there may be other explanations, as discussed in Ref. [15], focusing on the interpolation regime when the training error has already reached zero but boosting further still leads to testing error improvement (better generalisation). The combination of large trees focusing on extremely local neighbourhoods of the training dataset and averaging over a large number of trees seems to prevent overfitting efficiently. This has been interpreted in the more general framework of double descent risk curve [16]. With boosting, the interpolating regime behaviour (see Fig. 3(d)) may kick in even before the interpolating threshold, possibly explaining why typical boosted decision tree training curves look like Fig. 3(c).

4.4. Gradient boosting

While trying to understand how AdaBoost and other boosting algorithms work, they were originally recast in the statistical framework of arcing algorithms (an acronym for adaptive reweighting and combining) [34, 35]. At each step, a weighted minimisation is performed followed by a recomputation of the classifier and weighted input. This was further developed to become gradient boosting [30]. Boosting is formulated as a numerical optimisation problem, trying to minimise the loss function by adding trees
using a gradient descent procedure rather than giving a higher weight to misclassified events.

Formally, consider a model $F$ built iteratively, its imperfect instance at step $k$ being $F_k$. $F_k$ is therefore an approximation of the best possible model (in some cases $F_k(x) \neq y$), which is to be improved at the next iteration. This is achieved by adding a new component $h_k$ such that:

$$F_{k+1}(x) = F_k(x) + h_k(x) = y,$$

or equivalently:

$$h_k(x) = y - F_k(x).$$

Rather than training $F_{k+1}$ a new classifier can be trained to fit the residual $y - F_k(x)$, which corresponds to the part that the current model $F_k$ cannot treat correctly. If $F_{k+1}(x)$ is still not satisfactory, new iterations can be fitted.

The link with gradient descent is explicit when considering the particular case of the mean squared error (MSE) loss function (a typical case for regression problems, see Sec. 4.7):

$$L_{\text{MSE}}(x,y) = \frac{1}{2} (y - F_k(x))^2.$$  

Minimising the loss $J = \sum_i L_{\text{MSE}}(x_i, y_i)$ by adjusting all $F_k(x_i)$ leads to:

$$\frac{\partial J}{\partial F_k(x_i)} = \frac{\partial L_{\text{MSE}}(x_i, y_i)}{\partial F_k(x_i)} = F_k(x_i) - y_i.$$

Residuals can therefore be interpreted as negative gradients:

$$h_k(x_i) = y_i - F_k(x_i) = -\frac{\partial J}{\partial F_k(x_i)}.$$  

The concept can be generalised to any differentiable loss function instead of MSE. For instance AdaBoost corresponds to an exponential loss $e^{-F_k(x)y}$.

There are several variants of gradient boosting algorithms on the market. Techniques presented in Sec. 5 with subsampling of the training set and tree parameters can be used (in particular a bagging-like approach without replacement), leading to stochastic gradient boosting [36]. These regularisation techniques help prevent overfitting.

### 4.5. Boosting examples

The examples of this section illustrate typical behaviours of boosted decision trees.
4.5.1. The XOR problem

The XOR problem is a small version of the checkerboard, illustrated in Fig. 8. With enough statistics (Fig. 8(a) and Fig. 8(c)), even a single tree is already able to find more or less the optimal separation, so boosting cannot actually do much better.

The exercise can be repeated, this time with limited statistics (Fig. 8(b) and Fig. 8(d)). Now a single tree is not doing such a good job anymore. Boosted decision trees, on the other hand, are doing almost as well as with full statistics, separating almost perfectly signal and background. This illustrates very clearly how the combination of weak classifiers (see for instance the lousy performance of the first tree) can generate a high performance discriminant with a boosting algorithm.

4.5.2. Number of trees and overtraining

This example uses a highly correlated dataset, shown in Fig. 9(a).

Figure 9(b) compares the performance of a single decision tree and boosted decision trees with an increasing number of trees (from 5 to 400). All other parameters are kept to their default value in the TMVA package [37]. The performance of the single tree is not so good, as expected since the default parameters make it very small, with a depth of 3 (it should be noted that a single bigger tree could solve this problem easily). Increasing the number of trees improves the performance until it saturates in the high background rejection and high signal efficiency corner. Adding more trees does not seem to degrade the performance, the curve stays in the optimal corner. Looking at the contours in Fig. 9(a) it wiggles a little for larger boosted decision trees, as they tend to pick up features of the training sample. This is overtraining.

Another sign of overtraining also appears in Fig. 10, showing the output of the various boosted decision trees for signal and background, both on the training and testing samples: larger boosted decision trees tend to show differences between the two samples (as quantified by a Kolmogorov–Smirnov (KS) test in the figures, especially Fig. 10(f)), as they adjust to peculiarities of the training sample that are not found in an independent testing sample. The output acquires a ‘better’ shape with more trees, really becoming quasi-continuous, which would allow to cut at a precise efficiency or rejection.

Both figures do exhibit clear signs of overtraining, but is it really an issue? As mentioned before (see Sec. 2.6) what really matters in the end
is the performance in data analysis and on the testing sample. One way to evaluate this is to compute the maximum significance $s/\sqrt{s+b}$ (see Sec. 2.5.2). It is shown in Fig. 11(a) for the same boosted decision trees as shown in Fig. 10, with increasing number of trees. The best significance is actually obtained with the 400-tree boosted decision tree, following what was described at the end of Sec. 4.3. To be fair, the performance is very similar already with 10 trees. Now, comparing the outputs in Fig. 10, if interested in a smoother result, 10 trees might not be enough, but 50 would probably do, without the overhead of eight times more trees. Such a choice should in any case not be made based on overtraining statements comparing performance on the training and testing samples (as some are
Fig. 9. (a) 2D dataset and decision contour corresponding to several discriminants. (b) Background rejection vs. signal efficiency curves for a single decision tree (dark green) and boosted decision trees with an increasing number of trees (5 to 400).

tempted to do, seeing an increasing disagreement, quantified by the KS test, between outputs on the training and testing samples), but rather on final expected physics performance (the final number of the analysis, for instance the significance from the complete statistical analysis, possibly including systematic uncertainties). Boosted decision trees are often in the situation described in Fig. 3(c), meaning that their performance is not decreasing when boosting longer, even as the discrepancy in performance between train and test keeps increasing.

This example also illustrates the performance of each tree in a boosting sequence. Figure 11(b) shows the rapid decrease of the weight $\alpha_k$ of each tree, while at the same time the corresponding misclassification rate $\varepsilon_k$ of each individual tree increases rapidly towards just below 50%, that is, random guessing (Fig. 11(c)). It confirms that the best trees are the first ones, while the others are only minor corrections.

4.6. Other boosting algorithms

AdaBoost is but one of many boosting algorithms. It is also referred to as discrete AdaBoost to distinguish it from other AdaBoost flavours. The Real AdaBoost algorithm [31] defines each decision tree output as:

$$T_k(i) = 0.5 \times \ln \frac{p_k(i)}{1 - p_k(i)}.$$
Fig. 10. Comparison of the output on training (markers) and testing (histograms) signal (blue) and background (red) samples for boosted decision trees with 1, 5, 10, 50, 100 and 400 trees (from top left to bottom right). The Kolmogorov–Smirnov test quantifies the (dis)agreement between training and testing outputs.

Fig. 11. (a) Maximum significance of all boosted decision trees. (b) Boost weight of each tree. (c) Error fraction of each tree (0.5 means random guessing).

where \( p_x(i) \) is the purity of the leaf on which event \( i \) falls. Events are reweighted as:

\[ w_i^k \to w_i^{k+1} = w_i^k \times e^{-y_i T_k(i)} \]

and the boosted result is \( T(i) = \sum_{k=1}^{N_{\text{tree}}} T_k(i) \). Gentle AdaBoost and LogitBoost (with a logistic function) \cite{31} are other variations.
$\varepsilon$-Boost, also called shrinkage [30], consists in reweighting misclassified events by a fixed factor $e^{2\varepsilon}$ rather than the tree-dependent $\alpha_k$ factor of AdaBoost. $\varepsilon$-LogitBoost [31] is reweighting them with a logistic function $e^{-y_i T_k(i)}/(1 + e^{-y_i T_k(i)})$. $\varepsilon$-HingeBoost [2] is only dealing with misclassified events:

$$w_i^k \rightarrow w_i^{k+1} = \mathbb{I}(y_i \times T_k(i) \leq 0).$$

Finally the adaptive version of the ‘boost by majority’ [26] algorithm is called BrownBoost [38]. It works in the limit where each boosting iteration makes an infinitesimally small contribution to the total result, modelling this limit with the differential equations that govern Brownian motion.

4.7. Boosted regression trees

From their very introduction [6], trees have been considered for classification (decision trees) and for regression (regression trees), where instead of identifying ‘signal-like’ or ‘background-like’ regions of phase space, tree leaves each contain a single real value supposed to approach the target function.

During tree building for regression, the maximisation of the decrease of impurity in decision trees is replaced by the reduction of the standard deviation or of the mean squared error:

$$d(t) = \frac{1}{N_t} \sum_{N_t} (y - \hat{y}_t)^2,$$

for a node $t$ with $N_t$ events, regression target $y$ of each event in the node and mean value $\hat{y}_t$ of regression targets of all events in the node. Another typical choice for $d$ is the mean absolute error:

$$\frac{1}{N_t} \sum_{N_t} |y - \text{median}(y)_t|.$$

Constructing a regression tree is about finding the attribute that return the highest reduction in $d$ (i.e., the most homogeneous nodes) when going from node $t$ to nodes $t_P$ and $t_F$ (see Sec. 3.3 for notations):

$$\Delta d(S, t) = d(t) - p_P \cdot d(t_P) - p_F \cdot d(t_F).$$

The splitting stops when nodes become too small or when their internal variation is sufficiently small. The regression tree output is the mean (or median if using the mean absolute error) value of the training events in the corresponding (leaf) node. So a regression tree partitions the feature space
of input variables into hyperrectangles and then fits a constant inside each box.

When boosting regression trees, there are no longer properly and wrongly classified events, so the misclassification rate cannot be computed to reweight events. Instead the average loss $\langle L^k \rangle$ after the $k^{th}$ tree is computed over the training sample, and the boosting quantity $\beta_k = \langle L^k \rangle / (1 - \langle L^k \rangle)$ is derived. The reweighting of events is then computed based on their individual loss $L^k(i)$:

$$w_i^k \rightarrow w_i^{k+1} = w_i^k \times \beta_k^{1-L^k(i)}.$$ 

The training process is then similar to that of boosted decision trees, and the final prediction of the fitted value is the weighted average of all tree outputs.

4.8. Boosted decision trees in high-energy physics

Boosted decision trees have become very popular in high-energy physics. A few usage examples are presented in Sec. 4.8.1. Their proper usage also means addressing issues linked to systematic uncertainties, as reported in Sec. 4.8.2.

4.8.1. Use cases

The MiniBooNe experiment at Fermilab, searching for neutrino oscillations, was the first in the field to compare the performance of different boosting algorithms and artificial neural networks for analysis and particle identification [1, 2], on Monte Carlo samples. Trees with up to 120 variables were tested, with different boosting algorithms and up to thousands of trees. These studies introduced boosted decision trees in the particle physics world.

The concept of boosted decision trees was picked up by the D0 experiment at Fermilab, leading to the first evidence (and then observation) of single top quark production in Tevatron data [3, 4]. Among the 49 variables used, some had very similar definitions (like the scalar sum of transverse momentum of various jets), which was beneficial as not all of them suffer from the same mismeasurements on an event-by-event basis. Boosted decision trees happened to perform slightly better than two other techniques used: the matrix element calculation and Bayesian neural networks. Without such advanced techniques, the signal could not have been seen with the
dataset available at the time: the total uncertainty on the model prediction was much larger than the expected signal, as illustrated in Fig. 12(a). This also means that no single distribution (apart from the boosted decision tree output shown in Fig. 12(b)) could really show the new observed process, leading to scepticism in the community (‘I want to see a mass peak!’ is a common argument, reflecting on the fact that people are more confident in the result if they can see the signal in a physical distribution). Various cross-checks were performed to increase the degree of belief in the final outcome (removing top-quark-mass-related variables during training, validating the description of the boosted decision tree output in regions depleted in signal, analysing the shape of other variables after selecting low or high boosted decision tree output events enriched in background or signal events as shown in Fig. 12(c) and Fig. 12(d), respectively, etc.).

Since then, boosted decision trees have become a bread and butter technique in high energy physics and are extensively used in physics analyses (to extract their tiny signal from large backgrounds or distinguish between different signals) and object identification at the Tevatron or the LHC. In the ATLAS experiment $\tau$-lepton identification [39] and flavour tagging [7] used boosted decision trees in Run 2, and the $\tau$-lepton energy is estimated with boosted regression trees. The LHCb trigger was reoptimised, comparing the performance of several tree-based algorithms to neural networks [40], while their muon identification performance for the Run 3 of the LHC will profit from improvements thanks to gradient boosting [41].

The latest result has just been published at the time of writing, reporting the first evidence for $t\bar{t}t\bar{t}$ production in ATLAS [8], shown in Fig. 1(b). The one analysis using the most boosted decision trees is probably the observation of the diphoton decay of the Higgs boson by the CMS experiment [42]. The diphoton vertex is selected with a boosted decision tree, while another one estimates, event-by-event, the probability for the vertex assignment to be within 10 mm of the diphoton interaction point. Photons are identified with a boosted decision tree, and their energy is corrected with a boosted regression tree that provides the energy and its associated uncertainty. Finally several boosted decision trees are used to select the various signal regions and extract signal from these different categories.

Beyond object identification and calibration, and final discriminant in physics analyses, boosted decision trees can also be used to reduce the number of potential object combinations in order to find the correct match between the observed objects in the detector and their probable source of production. Such a ‘reconstruction BDT’ was used to look for the associated
production of a Higgs boson and a pair of top quarks, $t\bar{t}H(b\bar{b})$ [43].

Lately there is a tendency towards deep neural networks and their many flavours to replace boosted decision trees in the various stages of analysis [44, 45]. Boosted decision trees nevertheless remain a favourite in high-energy physics, for their ease of use, high performance out-of-the-box, limited required tuning of hyperparameters and resilience against overtraining.
4.8.2. Systematic uncertainties

There is an a priori, especially among physicists not very familiar with machine learning techniques, to distrust their output because they are not a measurable quantity with a physical meaning like an invariant mass. They are indeed complex variables, but so are for instance energy quantities for reconstructed particles in the detector. Uncertainties on such ‘basic’ variables are typically evaluated by varying the value of a requirement, changing the calibration of objects that go into the variable, etc. The boosted decision tree output (or of any such multivariate technique) is no different: its inputs can be varied according to their know uncertainties (for instance varying the jet energy scale will have a correlated impact on all discriminating variables that depend on jets) and their effect propagated through the boosted decision tree (the shifted inputs will lead to a different boosted decision tree output), to see how much these changes impact the analysis. This gives the size of the uncertainty on the multivariate discriminant output.

That being said, the Peter Parker principle applies: ‘With great power comes great responsibility’. Boosted decision trees are very powerful, and will target small areas of phase space where potentially not all known systematic uncertainties are strictly valid. Then extra uncertainties may be needed, not so much on the technique itself but rather due to the fact that it extracts information from less well-known regions.

Usually boosted decision trees are trained on the nominal Monte Carlo samples and are therefore completely oblivious to the effect of systematic uncertainties. This could lead to bad results once they are introduced, if the boosted decision trees are sensitive to them, and when applied on real data. One way to possibly mitigate this effect is with one form of data augmentation, training the boosted decision trees on a mixture of nominal and systematically shifted events, hence increasing the training statistics and allowing the boosted decision trees to see other events than the nominal ones during training to learn their features. The nominal performance should decrease, but with the hope that systematic uncertainties will have less of an impact on the final measurement. Experience with this approach is inconclusive. If the physics model is not properly describing the real data, then the performance will also be affected. It can be partially addressed with domain adaptation [5] (as described elsewhere in this book).
5. Other averaging techniques

As mentioned in Sec. 3.5.3 the key to improving a single decision tree performance and stability is averaging. Other techniques than boosting exist, some of which are briefly described below. As with boosting, statistical perturbations are introduced to randomise the training sample, hence increasing the predictive power of the ensemble of trees.

**Bagging** (Bootstrap AGGregatING) was proposed in Ref. [46]. It consists in training trees on different bootstrap samples drawn randomly with replacement from the training sample. Events that are not picked for the bootstrap sample form an ‘out of bag’ validation sample. The bagged output is the simple average of all such trees, with a reduced variance compared to individual trees.

**Random forests** is bagging with an extra level of randomisation [20]. Before splitting a node, only a random subset of discriminating variables is considered. The fraction can vary for each split for yet another level of randomisation.

**Trimming** is not exactly an averaging technique per se but can be used in conjunction with another technique, in particular boosting, to speed up the training process. After some boosting cycles, it is possible that very few events with very high weight are making up most of the total training sample weight. Events with very small weights may be ignored, hence introducing again some minor statistical perturbations and speeding up the training. ε-HingeBoost is such an algorithm (see Sec. 4.6).

6. Software

Many implementations of decision trees exist on the market. Some of them, all open source, are briefly presented below.

The most popular in high-energy physics is TMVA [37], integrated into ROOT. It includes single decision trees, boosted trees with AdaBoost and gradient boost, bagging and random forests. Being part of ROOT it is very straightforward to use within usual analysis frameworks, both in C++ and Python. It includes tools for data preparation and makes it simple to compare performance between many algorithms, not only tree-based ones. Already mentioned Refs. [7, 8, 39, 42, 43] are but a few examples of TMVA usage in the field.
Another implementation has gained visibility in high-energy physics: XGBoost [47]. It entered the field after receiving a special HEP meets ML award during the Higgs boson machine learning challenge (HiggsML) hosted by Kaggle [11] (described in Chapter 20). It features a high-performing, scalable gradient boosting implementation, capable of using GPU and large cluster parallelisation. Instead of the greedy algorithm described in Sec. 3.1, the authors developed an approximate algorithm that proposes candidate splitting points according to percentiles of the input variables, and then maps the variables into buckets according to these splits to find the best solution. Many analyses at the LHC are now using it (see for instance Ref. [48]).

Other implementations have lower usage in high-energy physics so far while being used in other fields. LightGBM (light gradient boosting machine [49]), originally developed by Microsoft, is competing with XGBoost in speed, scalability and performance. It builds trees in a very different way from what was presented in this chapter, with a histogram-based decision tree learning algorithm. Scikit-learn [50] is a very popular machine learning framework with several tree-related implementations and utilities for data preparation. Finally CatBoost [51] is a new gradient boosting implementation from Yandex used in commercial services as well as in high-energy physics, for instance in LHCb [41].

7. Conclusion

This chapter introduced what decision trees are and how to construct them, as a powerful multivariate extension of a cut-based analysis. Advantages are numerous: their training is fast, they lead to human-readable results (not black boxes) with possible interpretation by a physicist, can deal easily with all sorts of variables and with many of them, with in the end relatively few parameters.

Decision trees are, however, not perfect and suffer from the piecewise nature of their output and a high sensitivity to the content of the training sample. These shortcomings are for a large part addressed by averaging the results of several trees, each built after introducing some statistical perturbation in the training sample. Among the most popular such techniques, boosting (and its AdaBoost and gradient boost incarnations) was described in detail, providing ideas as to why it seems to be performing so well while being very resilient against overtraining. Other averaging techniques were briefly presented.
Boosted decision trees have now become quite fashionable in high energy physics. Following the steps of MiniBooNe for analysis and particle identification and D0 for the first evidence and observation of single top quark production, other experiments and analyses are now using them routinely, in particular at the LHC.

Boosted decision trees are still a very active field of development, with academic groups and private companies testing their limits, providing new software [47, 49, 51] and using them to target recent issues like resistance to adversarial attacks (see e.g. [52, 53]).

References

[1] B. P. Roe et al., Boosted decision trees as an alternative to artificial neural networks for particle identification, Nucl. Instr. Meth. A 543 (2005) 577.
[2] H.-J. Yang, B. P. Roe, and J. Zhu, Studies of boosted decision trees for MiniBooNE particle identification, Nucl. Instr. Meth. A 555 (2005) 370.
[3] D0 Collaboration, Evidence for Production of Single Top Quarks and First Direct Measurement of $|V_{tb}|$, Phys. Rev. Lett. 98 (2007) 181802.
[4] D0 Collaboration, Evidence for production of single top quarks, Phys. Rev. D 78 (2008) 012005.
[5] S. Ben-David et al., A theory of learning from different domains, Mach. Learn. 79 (2009) 151.
[6] L. Breiman, J. H. Friedman, R. A. Olshen, and C. J. Stone, Classification and Regression Trees. Wadsworth, 1984.
[7] ATLAS Collaboration, ATLAS b-jet identification performance and efficiency measurement with $t\bar{t}$ events in pp collisions at $\sqrt{s} = 13$ TeV, Eur. Phys. J. C 79 (2019) 970, arXiv:1907.05120 [hep-ex].
[8] ATLAS Collaboration, Evidence for $t\bar{t}t\bar{t}$ production in the multilepton final state in proton–proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector, Eur. Phys. J. C 80 (2020) 1085, arXiv:2007.14858 [hep-ex].
[9] G. Cowan et al., Asymptotic formulae for likelihood-based tests of new physics, Eur. Phys. J. C 71 (2011) 1554, arXiv:1007.1727 [physics.data-an]. Erratum: Eur. Phys. J. C 73 (2013) 2501.
[10] L. Moneta et al., The RooStats project, PoS ACAT2010 (2011) 057, arXiv:1009.1003 [physics.data-an].
[11] C. Adam-Bourdarios et al., The Higgs boson machine learning challenge, in Proceedings of the NIPS 2014 Workshop on High-energy Physics and Machine Learning, 2015.
[12] T. Hastie, R. Tibshirani, and J. Friedman, The Elements of Statistical Learning: Data Mining, Inference, and Prediction (2nd edition). Springer Series in Statistics. Springer, 2009.
https://web.stanford.edu/~hastie/ElemStatLearn/.
[13] T. Hastie, R. Tibshirani, and M. Wainwright, Statistical Learning with Sparsity: The Lasso and Generalizations. Chapman & Hall/CRC
Monographs on Statistics and Applied Probability, 2015.  
https://web.stanford.edu/~hastie/StatLearnSparsity/.

[14] N. Srivastava et al., Dropout: A Simple Way to Prevent Neural Networks from Overfitting, J. Mach. Learn. Res. 15 (2014) 1929–1958.

[15] A. J. Wyner, M. Olson, J. Bleich, and D. Mease, Explaining the Success of AdaBoost and Random Forests as Interpolating Classifiers, J. Mach. Learn. Res. 18 (2017) 1.

[16] 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].

[17] I. Kononenko, Machine learning for medical diagnosis: history, state of the art and perspective, Artif. Intell. Med. 23 (2001) 89.

[18] V. Podgorelec, P. Kokol, B. Stiglic, and I. Rozman, Decision Trees: An Overview and Their Use in Medicine, J. Med. Syst. 26 (2002) 445.

[19] C. Gini, Variabilità e mutabilità, (reprinted in Memorie di Metodologia Statistica, eds. E. Pizetti and T. Salvemini, Libreria Eredi Virgilio Veschi, Rome, 1955), 1912.

[20] L. Breiman, Random forests, Mach. Learn. 45 (2001) 5.

[21] S. Shalev-Shwartz and S. Ben-David, Understanding Machine Learning: From Theory to Algorithms. Cambridge University Press, 2014.  
https://www.cs.huji.ac.il/~shais/UnderstandingMachineLearning.

[22] J. R. Quinlan, Simplifying decision trees, Int. J. Man-Mach. Stud. 27 (1987) 221.

[23] J. H. Friedman and B. E. Popescu, Predictive learning via rule ensembles, Ann. Appl. Stat. 2 (2008) 916, arXiv:0811.1679 [stat.AP].

[24] T. G. Dietterich, Machine learning research: Four current directions, AI Magazine 18 (1997) 97.

[25] R. E. Schapire, The strength of weak learnability, Mach. Learn. 5 (1990) 197.

[26] Y. Freund, Boosting a Weak Learning Algorithm by Majority, Inf. Comput. 121 (1995) 256.

[27] Y. Freund and R. E. Schapire, Experiments with a New Boosting Algorithm, in Proceedings of the Thirteenth International Conference on Machine Learning, ICML’96. 1996.

[28] Y. Freund and R. E. Schapire, A Decision-Theoretic Generalization of On-Line Learning and an Application to Boosting, J. Comput. Syst. Sci. 55 (1997) 119.

[29] R. E. Schapire and Y. Freund, Boosting: Foundations and Algorithms. MIT Press, 2012.

[30] J. H. Friedman, Greedy function approximation: A gradient boosting machine., Ann. Statist. 29 (2001) 1189.

[31] J. H. Friedman, T. Hastie, and R. Tibshirani, Additive logistic regression: a statistical view of boosting. Ann. Statist. 28 (2000) 337.

[32] R. E. Schapire, Y. Freund, P. Bartlett, and W. S. Lee, Boosting the margin: a new explanation for the effectiveness of voting methods, Ann. Statist. 26 (1998) 1651.
[33] V. N. Vapnik, *The Nature of Statistical Learning Theory*, Springer, 2000.
[34] L. Breiman, *Arcing the Edge*, Ann. Prob. 26 (1998) 1683.
[35] L. Breiman, *Prediction Games and Arcing Algorithms*, Neural Comput. 11 (1999) 1493.
[36] J. H. Friedman, *Stochastic gradient boosting*, Comput. Stat. Data Anal. 38 (2002) 367.
[37] A. Hoecker et al., *TMVA — Toolkit for Multivariate Data Analysis*, arXiv:physics/0703039 [physics.data-an].
[38] Y. Freund, *An Adaptive Version of the Boost by Majority Algorithm*, Mach. Learn. 43 (2001) 293–318.
[39] ATLAS Collaboration, *Measurement of the tau lepton reconstruction and identification performance in the ATLAS experiment using pp collisions at √s = 13 TeV*, ATLAS-CONF-2017-029, 2017.
[40] T. Likhomanenko et al., *LHCb Topological Trigger Reoptimization*, J. Phys. Conf. Ser. 664 (2015) 082025, arXiv:1510.00572 [physics.ins-det].
[41] L. Anderlini et al., *Muon identification for LHCb Run 3*, arXiv:2008.01579 [hep-ex].
[42] CMS Collaboration, *Observation of the di-photon decay of the Higgs boson and measurement of its properties*, Eur. Phys. J. C 74 (2014) 3076, arXiv:1407.0558 [hep-ex].
[43] ATLAS Collaboration, *Search for the standard model Higgs boson produced in association with top quarks and decaying into a b¯b pair in pp collisions at √s = 13 TeV with the ATLAS detector*, Phys. Rev. D 97 (2018) 072016, arXiv:1712.08895 [hep-ex].
[44] ATLAS Collaboration, *Identification of hadronic tau lepton decays using neural networks in the ATLAS experiment*, ATL-PHYS-PUB-2019-033, 2019.
[45] ATLAS Collaboration, *Deep Sets based Neural Networks for Impact Parameter Flavour Tagging in ATLAS*, ATL-PHYS-PUB-2020-014, 2020.
[46] L. Breiman, *Bagging predictors*, Mach. Learn. 24 (1996) 123.
[47] T. Chen and C. Guestrin, *XGBoost: A Scalable Tree Boosting System*, in Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD ’16. Association for Computing Machinery, 2016. arXiv:1603.02754 [cs.LG].
[48] ATLAS Collaboration, *Observation of Higgs boson production in association with a top quark pair at the LHC with the ATLAS detector*, Phys. Lett. B 784 (2018) 173, arXiv:1806.00425 [hep-ex].
[49] G. Ke et al., *LightGBM: A Highly Efficient Gradient Boosting Decision Tree*, in Advances in Neural Information Processing Systems, 2017.
[50] F. Pedregosa et al., *Scikit-learn: Machine learning in Python*, J. Mach. Learn. Res. 12 (2011) 2825.
[51] A. V. Dorogush, V. Ershov, and A. Gulin, *CatBoost: gradient boosting with categorical features support*, arXiv:1810.11363 [cs.LG].
[52] H. Chen et al., *Robustness Verification of Tree-based Models*, in Advances in Neural Information Processing Systems. 2019.
and trees against adversarial attacks, in *Advances in Neural Information Processing Systems*. 2019.