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New approaches for boosting to uniformity

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ABSTRACT: The use of multivariate classifiers has become commonplace in particle physics. To enhance the performance, a series of classifiers is typically trained; this is a technique known as boosting. This paper explores several novel boosting methods that have been designed to produce a uniform selection efficiency in a chosen multivariate space. Such algorithms have a wide range of applications in particle physics, from producing uniform signal selection efficiency across a Dalitz-plot to avoiding the creation of false signal peaks in an invariant mass distribution when searching for new particles.

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Contents

1. Introduction

Methods of machine learning play an important role in modern particles physics. Multivariate classifiers, *e.g.*, boosted decision trees (BDTs) and artificial neural networks (ANNs), are now commonly used in analysis selection criteria. BDTs are now even used in software triggers [1, 2]. To enhance the performance, a series of classifiers is typically trained; this is a technique known as boosting. Boosting involves training many simple classifiers and then building a single composite classifier from their responses. The classifiers are trained in series with the inputs of each member being augmented based on the performance of its predecessors. This augmentation is designed such that each new classifier targets more those events which were poorly classified by previous members of the series. The classifier obtained by combining all members of the series is typically much more powerful than any of the individual members.

In particle physics, the most common usage of BDTs is in classifying candidates as signal or background. The BDT is determined by optimizing some figure of merit (FOM), *e.g.*, the signal purity or approximate signal significance. This approach is optimal for a counting experiment; however, in many cases the BDT-based selection obtained in this way is not optimal. For example, in a Dalitz-plot (or any angular or amplitude analysis) analysis, obtaining a selection efficiency

on signal candidates that is uniform across the Dalitz-plot is more important than any integrated FOM. Similarly, when measuring a mean particle lifetime, obtaining an efficiency that is uniform in lifetime is what is desired. In both cases, obtaining a uniform selection efficiency greatly reduces the systematic uncertainties involved in the measurement. When searching for a new particle, an analyst may want a uniform efficiency in mass for selecting background candidates so that the BDT-based selection does not generate a fake signal peak. Furthermore, the analyst may also desire a uniform selection efficiency of signal candidates in mass (or other variates) since the new particle mass is not known. In such cases, the BDT is often trained on simulated data generated with several values of mass (lifetime, *etc.*). A uniform selection efficiency in mass ensures that the BDT is sensitive to the full range of masses involved in the search.

2. Uniformity Boosting Methods

The variates used in the BDT are denoted by $\vec{x}$, while the variates in which uniformity is desired are denoted by $\vec{y}$. Some (perhaps all) of the $\vec{x}$ variantes will be *biasing* in $\vec{y}$, *i.e.* they provide discriminating power between signal and background that varies in $\vec{y}$. A uniform BDT selection efficiency can be obtained by removing all such variates; however, this will also reduce the power of the BDT. The goal of boosting algorithms presented in this paper is to *balance* the biases to produce the optimal uniform selection.

One category of boosting works by assigning training events more weight based on classification erros made by previous members of the series. For example, the AdaBoost [**?**] algorithm updates the weight of event i, w_i, according to

$$w_i' = w_i \times \exp\left[-\gamma_i p_i\right], \tag{2.1}$$

where $\gamma = +1(-1)$ for signal(background) events and p is the prediction for each event produced by last classifier in the series. The uBoost technique, described in detail in Ref. [**?**], alters the event-weight updating procedure to achieve uniformity in the signal-selection efficiency.

Another approach to obtain uniformity, introduced in this paper, involves defining a more general expression of the AdaBoost criteria:

$$w_i' = w_i \times \exp\left[-\gamma_i \sum_j a_{ij} p_j\right], \tag{2.2}$$

where a_{ij} are the elements of some matrix A[1]. For the case where A is the identity matrix, the AdaBoost weighting procedure is recovered. Other choices of A will induce non-local effects, *e.g.*, consider the sparse matrix A_{knn} given by

$$a_{ij}^{\text{knn}} = \begin{cases} \frac{1}{k}, & j \in \text{knn}(i), \text{ events } i \text{ and } j \text{ belong to the same class} \\ 0, & \text{otherwise,} \end{cases} \tag{2.3}$$

where $\text{knn}(i)$ denotes the set of k-nearest-neighbor events to event i. This procedure for updating the event weights, which we refer to as kNNAdaBoost, accounts for the score of each event's k nearest neighbors and not just each event individually.

[1] A natural choice is a square $n \times n$ matrix, but this is not required.

The gradient boosting [**?**] (GB) algorithm category requires the analyst to choose a differentiable loss function with the goal of building a classifier that minimizes the loss. A popular choice of loss function is the AdaLoss [**?**] function

$$L_{\text{ada}} = \sum_{i=1}^{n} \exp\left[-\gamma_i s_i\right]. \tag{2.4}$$

So-called scores s are obtained for each event as sum of predictions of all regressots in the series At each stage in the gradient boosting process, a *regressor* (a decision tree in our case) is trained whose purpose is to decrease the loss. This is accomplished using the gradient decent method and the *pseudo-residuals*

$$-\frac{\partial L_{\text{ada}}}{\partial s_i} = \gamma_i \exp\left[-\gamma_i s_i\right], \tag{2.5}$$

which are positive(negative) for signal(background) events and have larger modulai for poorly classified events.

The gradient-boosting algorithm is general in that it only requires the analyst specify a loss function and its gradient. The AdaLoss function considers each event individually, but can easily be modified to take into account non-local properties of the classifier as follows:

$$L_{\text{general}} = \sum_{i=1}^{n} \exp\left[-\gamma_i \sum_j a_{ij} s_j\right]. \tag{2.6}$$

For example, the loss function obtained from Eq. 2.6 using A_{knn}, which we refer to as kNNAdaLoss and denote L_{knn}, accounts for the score of each event's k nearest neighbors and not just each event individually. The pseudo-residuals of L_{knn} are

$$-\frac{\partial L_{\text{knn}}}{\partial s_k} = \sum_i \gamma_i a_{ik}^{\text{knn}} \exp\left[-\gamma_i \sum_j a_{ij}^{\text{knn}} s_j\right]. \tag{2.7}$$

One can see that the direction of the gradient will be influenced the most by events whose k-nearest-neighbor events are classified poorly.

Another approach is to include in the definition of the loss function some uniformity metric. Consider first the case where the data have been binned in $\vec{y}$. If the distribution of classifier responses in each bin, $f_b(s)$, is the same as the global response distribution, $f(s)$, then any cut made on the response will produce a uniform selection efficiency in $\vec{y}$. Therefore, performing a one-dimensional goodness-of-fit test of the hypothesis $f_b \equiv f$ in each bin provides an assessment of the selection uniformity. For example, one could perform the Kolmogorov-Smirnov test in each bin and define a loss function as follows:

$$L_{\text{flat(KS)}} = \sum_b w_b \max|F_b(s) - F(s)|, \tag{2.8}$$

where $F_{(b)}(s)$ denotes the cumulative distribution of $f_{(b)}(s)$ and $w_b = \sum \delta(\text{bin}_i - b)/n_{\text{signal}}$, *i.e.* w_b is the fraction of signal events in the bin[2].

[2]If weighted events are used, then the fractional sum of weights should be used for w_b.

The gradient of the Kolmogorov-Smirnov loss function is zero for events with responses not equal to than the value of s at which $\max|F_b(s) - F(s)|$ occurs. Thus, it is not suitable for gradient boosting due to its instability. Instead, we use the following *flatness* loss function:

$$L_{\text{flat}} = \sum_b w_b \int |F_b(s) - F(s)|^2 ds, \tag{2.9}$$

whose pseudo-residuals are (b is bin containing kth event)

$$-\frac{\partial L_{\text{flat}}}{\partial s_k} \approx -2w_b \left[F_b(s_k) - F(s_k)\right]. \tag{2.10}$$

This so-called flatness loss penalizes non-uniformity but does not consider the quality of the classification. Therefore, the full loss function used is

$$L_{\text{ada+flat}} = L_{\text{flat}} + \alpha L_{\text{ada}}, \tag{2.11}$$

where α is a real-valued parameter that is typically chosen to be small. The first term in Eq. 2.11 penalizes non-uniformity, while that second term penalizes poor classification.

The loss function given in Eq. 2.11 can also be constructed without binning the data using k-nearest-neighbor events. The cumulative distribution $F_{\text{knn}}(s)$ is easily obtained and the bin weight, w_b, is replaced by a k-nearest-neighbor weight, w_{knn}. First, each event is weighted by the inverse of the number of times it is included in the k-nearest-neighbor sample of another event. Then, w_{knn} is the sum of such weights in a k-nearest-neighbor sample divided by the total sum of such weights in the full sample. This procedure is followed to offset the fact that some events are found in more k-nearest-neighbor samples than other events.

3. Example Analysis

The example analysis studied here involves a so-called Daltiz-plot analysis. In such analyses, the distribution of events in a 2-D space is typically fit to extract some information of physical interest. The regions of the Daltiz-plot that tend to have the highest sensitivity to the desired information are the *edges*. Unfortunately, the edge regions also typically have the most background contamination and the least discrimination against background. Therefore, traditional classifier-based selections tend to produce selections for Dalitz-plot analyses with lower efficiency near the edges.

This study uses simulated event samples produced using the official LHCb simulation framework. The software used for the generation of the events is described in LHCb publications as follows :

> In the simulation, pp collisions are generated using PYTHIA [4] with a specific LHCb configuration [5]. Decays of hadronic particles are described by EvtGen [6], in which final state radiation is generated using PHOTOS [7]. The interaction of the generated particles with the detector and its response are implemented using the GEANT toolkit [8, 9] as described in Ref. [10].

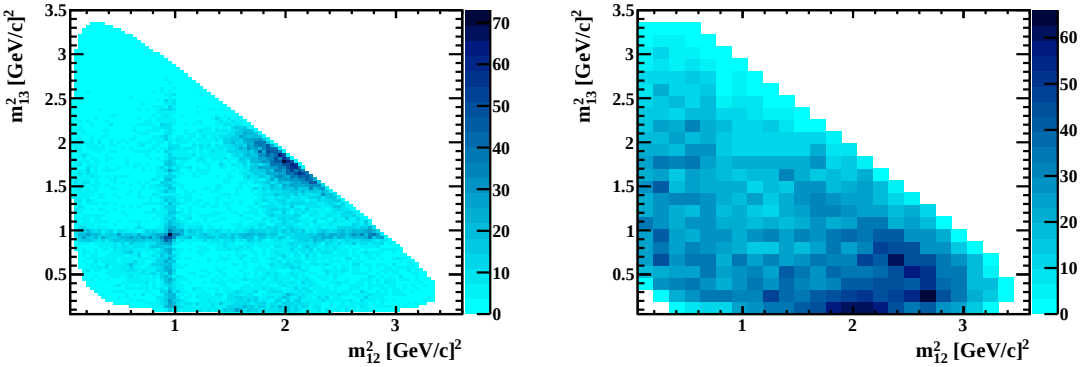

Figure 1: Dalitz-plot distributions for (left) signal and (right) background for the $D_s^{\pm} \to \pi^+\pi^-\pi^{\pm}$. The three pions are labeled here as 1, 2 and 3.

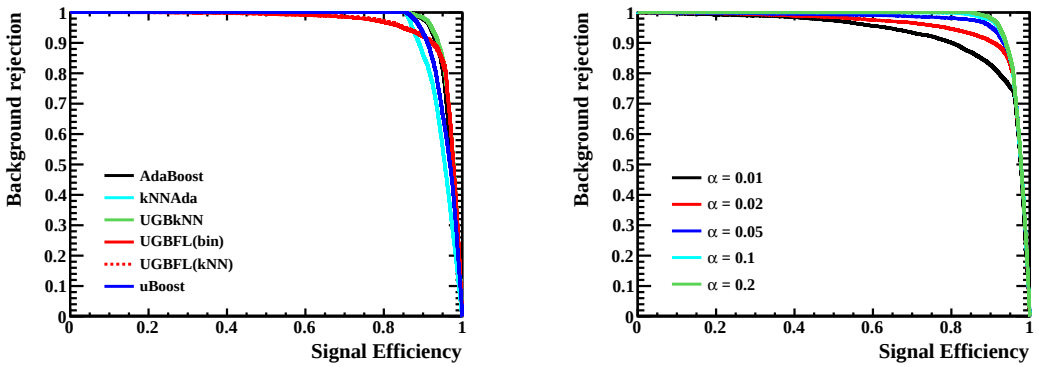

Figure 2: Efficiency *vs* distance to a corner of the Dalitz-plot. An arbitrary working point of 50% integrated efficiency is displayed.

All simulated event samples are generated inside the LHCb detector acceptance. The signal used in this analysis consists of $D_s^{\pm} \to \pi^+\pi^-\pi^{\pm}$ decays, simulated using the D_DALITZ model of EvtGen to simulate the intermediate resonances which contribute to the three pion final state. The background candidates are three pion combinations reconstructed in simulated samples of $c\bar{c}$ and $b\bar{b}$ events, where the charm and bottom quark decays are inclusively modelled by EvtGen. The simulated events contain "truth" information which identifies them as signal or background, and which identifies the physical origin of the three pion combinations reconstructed in the $c\bar{c}$ and $b\bar{b}$ simulated samples.

Figure 1 shows the Dalitz-plot distributions for signal and background events. These samples are split into training and testing samples and then various BDTs are trained. Figure 4 shows the efficiency obtained for each classifier *vs* distance from the a corner of the Dalitz-plot. The AdaBoost algorithm, as expected, produces a much lower efficiency in the interesting corner regions. The kNNAdaBoost algorithm does not improve upon the AdaBoost result much. This is likely due to the fact that while kNNAdaBoost uses non-local kNN information, it does not utilize global information. The UGBFL (binned and unbinned kNN) and uBoost algorithms each produce an efficiency which is statistically consistent with uniform across the Dalitz plot.

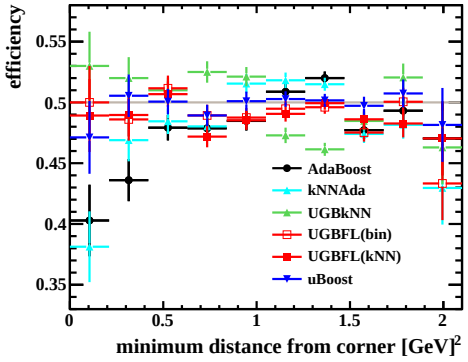

Figure 3: Efficiency *vs* distance to a corner of the Dalitz-plot. An arbitrary working point of 50% integrated efficiency is displayed.

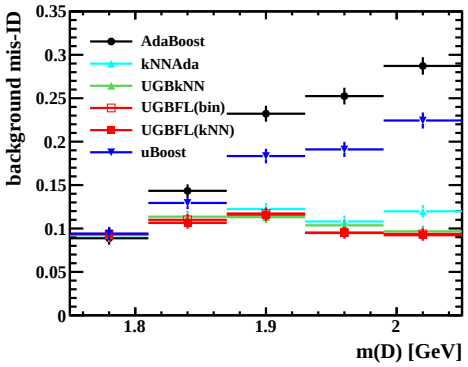

Figure 4: Background mis-identification *vs* D candidate mass for (black circles) AdaBoost, (cyan up triangles) kNNAdaBoost, (red filled squares) UGBFL(bin), (red open squares) UGBFL(knn), and (blue down triangles) uBoost. An arbitrary working point of 10% background mis-identification in the training region $1.75 < m(D) < 1.85$ GeV is displayed.

ADD DISCUSSION ON ROC CURVE HERE ...

4. Timings

The main drawback of uBoost technique is it's high computational complexity: while simple AdaBoost trains M trees, uBoost builds $100 \times M$ trees (contribution of other operations usually can be neglected).

Presented in this paper classifiers are building M trees, though there is more complicated boosting, it takes at each iteration (k is number of neighbors, N is number of events in training sample)

- meanAdaBoost: $O(k \times N)$
- knnAdaLoss: $O(k \times N)$, for the arbitrary matrix A it is $O(\#\text{nonzero elements in the matrix})$
- FlatnessLoss on bins: $O(N \ln N)$

- FlatnessLoss on knn: $O(N \ln N + Nk \ln k)$

5. Summary

6. Source code

The link on the repository ans links to final notebooks with results in the article.

Acknowledgments

These results were obtained using events generated with the official LHCb simulation, and we are grateful to the LHCb collaboration for this privilege. We particularly acknowledge the work of the LHCb Simulation and Core Computing teams in tuning the simulation software and managing the productions of simulated events.

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A. Measures of uniformity

In this section we discuss different methods for measuring the uniformity of prediction. One typical way of 'checking' uniformity of prediction used by physicists is fitting the distribution of the events that were classified as signal (or background) over the feature for which you wish to check uniformity. This approach requires assumptions about the shape of the distribution, which makes quantitative comparisons of different classifiers difficult. Our aim here is to explore uniformity figures of merit which make comparing classifiers easier, analogously to how the area under the ROC curve can be used to compare absolute classifier performance.

The output of event classification is the probability of each event being signal or background, and it is only after we apply a cut on this probability that events are classified. An ideal uniformity of signal prediction can then be defined for a given "uniform feature" of interest. It means that whichever cut we select, the efficiency for a signal event to pass the cut doesn't depend on the uniform feature. Uniformity for background can be defined in the same manner, but for simplicity, in what follows we will only discuss the uniformity of efficiency for signal events.

A trivial example of a classifier that has ideal uniformity is a classifier which returns a random classification probability, but such a classifier is of course not very useful. One can try to design a uniform classifier with respect to a given feature by not using this feature, or any correlated features, in the classification; in practice, however, this approach also tends to lead to poorly performing classifiers. The approach which we take in this paper is to explicitly let the classifier learn how to balance non-uniformities coming from different features in such a way as to generate a classification which is uniform on average. It is then important to be able to accurately measure the uniformity of classification.

Before proceeding, it is useful to define some desirable properties of uniformity metrics

1. The metric shouldn't depend strongly on the number of events used to test uniformity;
2. The metric shouldn't depend on the normalization of the event weights: if we multiply all the weights by some arbitrary number, it shouldn't change at all;
3. The metric should depend only on the order of predictions, not the exact values of probabilities. This is because we care about which events pass the cut and which don't, not about the exact values of predictions. For example: correlation of prediction and mass doesn't satisfy this restriction.
4. The metric should be stable against any of its own free parameters: if it uses bins, changing the number of bins shouldn't affect the result, if it uses k-nearest neighbors, it should be stable against different values of k.

In what follows we will consider different metrics which satisfy these criteria, and then compare their performance in some test cases.

A.1 Standard Deviation of Efficiency on Bins (SDE)

If the space of uniform features is split into bins, it is possible to define the global efficiency

$$\text{eff} = \frac{\text{total weight of signal events that passed the cut}}{\text{total weight of signal events}},$$

as well as the efficiency in every bin,

$$\text{eff}_{\text{bin}} = \frac{\text{weight of signal events in bin that passed the cut}}{\text{weight of signal events in this bin}}.$$

One measure of non-uniformity is the standard deviation of bin efficiencies from the global efficiency:

$$\sqrt{\sum_{\text{bin}} (\text{eff}_{\text{bin}} - \text{eff})^2}.$$

To make the metric more stable against fluctuations in bins which contain very few events, we add weights to the bins (note that $\sum_{\text{bin}} \text{weight}_{\text{bin}} = 1$):

$$\text{weight}_{\text{bin}} = \frac{\text{total weight of signal events in bin}}{\text{total weight of signal events}},$$

giving the weighted standard deviation (SDE) formula

$$\text{SDE}(\text{eff}) = \sqrt{\sum_{\text{bin}} \text{weight}_{\text{bin}} \times (\text{eff}_{\text{bin}} - \text{eff})^2}.$$

This formula is valid for any given cut value. To measure the overall non-flatness of the selection, we take several global efficiencies and use

$$\text{SDE}^2 = \frac{1}{k} \sum_{\text{eff} \in [\text{eff}_1 \ldots \text{eff}_k]} \text{SDE}^2(\text{eff})$$

Another power $p \neq 2$ can be used as well, but $p = 2$ is considered as the default value.

A.2 Theil Index of Efficiency

The Theil Index is frequently used to measure economic inequality:

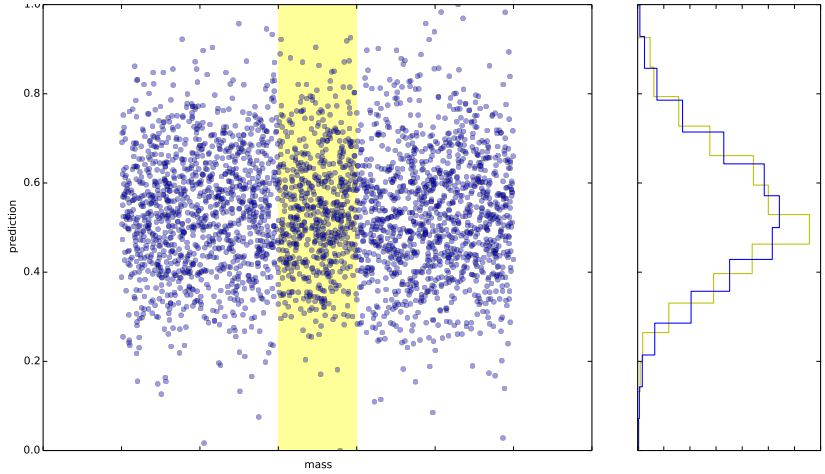
$$\text{Theil} = \frac{1}{N} \sum_i \frac{x_i}{< x >} \ln \frac{x_i}{< x >}, \qquad < x >= \frac{1}{N} \sum_i x_i$$

In our case we have to alter formula a bit to take into account that different bins have different impact, thus the formula turns into

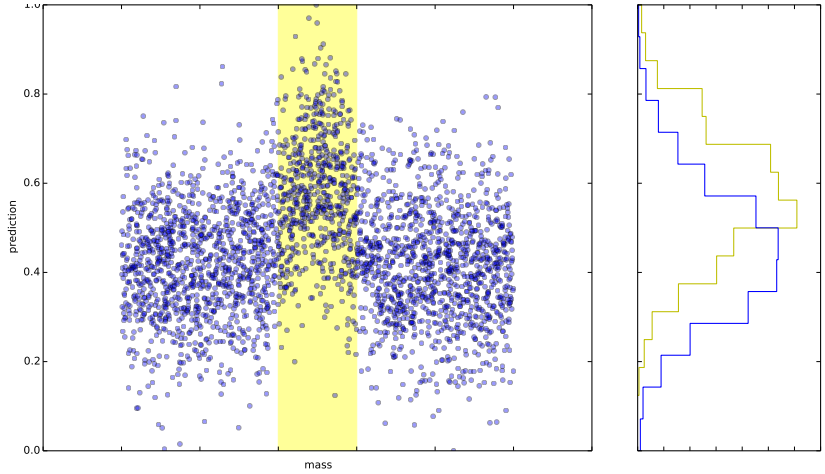
$$\text{Theil}(\text{eff}) = \sum_{\text{bin}} \text{weight}_{\text{bin}} \frac{\text{eff}_{\text{bin}}}{\text{eff}} \ln \frac{\text{eff}_{\text{bin}}}{\text{eff}}.$$

To measure the overall non-flatness, we average values for several global efficiencies:

$$\text{Theil} = \frac{1}{k} \sum_{\text{eff} \in [\text{eff}_1 \ldots \text{eff}_k]} \text{Theil}(\text{eff})$$



(a) Predictions are uniform in mass, the distribution of predictions in the bin (yellow) is close to the global (blue). Yellow rectangle shows the events in the bin over mass.



(b) Distribution with peak in the middle, the distribution in the bin is quite different from global.

Figure 5: Demonstration of distribution similarity approach.

A.3 Distribution Similarity Approach

Instead of measuring uniformity in terms of binned efficiencies, it is possible to consider the distribution of the binned classifier predictions, F_{bin}, directly. Ideal uniformity means that all the distributions F_{bin} are equal and hence equal to the global distribution $F(x)$. This is demonstrated on figure 5. To 'measure' non-flatness we can use some distribution distance, like Kolmogorov-Smirnov:

$$\sum_{\text{bin}} \text{weight}_{\text{bin}} \max_x |F_{\text{bin}}(x) - F(x)|,$$

but Cramér–von Mises similarity is more informative (usually $p = 2$ is used):

$$\sum_{\text{bin}} \text{weight}_{\text{bin}} \int |F_{\text{bin}}(x) - F(x)|^p \, dF(x),$$

in particular because Kolmogorov-Smirnov measures are too sensitive to local non-uniformities. The advantage of this method is that we don't need to select some global efficiencies like in the previous metrics.

A.4 Knn-based modifications

Though operating with bins is usually both simple and very efficient, in many cases it is hard to find the optimal size of bins in the space of uniform features (specifically in the case of more than two dimensions). As mentioned earlier, problems can also arise due to bins with very low populations.

In these cases we can switch to k-nearest neighbors: for each signal event we find k nearest signal events (including the event itself) in the space of uniform features. Now we can compute the efficiency $\text{eff}_{\text{knn}(i)}$, from the empirical distribution $F_{\text{knn}(i)}$ of nearest neighbors. The weights for $\text{knn}(i)$ are proportional to the total weight of events in $\text{knn}(i)$:

$$\text{weight}_{\text{knn}(i)} = \alpha \sum_{j \in \text{knn}(i)} w_j, \qquad \alpha^{-1} = \sum_i \sum_{j \in \text{knn}(i)} w_j,$$

so again weights are normed to 1: $\sum_i \text{weight}_{\text{knn}(i)} = 1$.

It is then possible to write the knn versions of SDE

$$\text{knnSDE}^2(\text{eff}) = \sum_{i \in \text{events}} \text{weight}_{\text{knn}(i)} \left|\text{eff}_{\text{knn}(i)} - \text{eff}\right|^2,$$

$$\text{knnSDE}^2 = \frac{1}{k} \sum_{\text{eff} \in [\text{eff}_1, \ldots \text{eff}_k]} \text{knnSDE}^2(\text{eff}),$$

the Theil index of efficiency

$$\text{knnTheil}(\text{eff}) = \sum_{i \in \text{events}} \text{weight}_{\text{knn}(i)} \, \frac{\text{eff}_{\text{knn}(i)}}{\text{eff}} \, \ln \frac{\text{eff}_{\text{knn}(i)}}{\text{eff}},$$

$$\text{knnTheil} = \frac{1}{k} \sum_{\text{eff} \in [\text{eff}_1, \ldots \text{eff}_k]} \text{knnTheil}(\text{eff}),$$

and the similarity-based measure:

$$\sum_{i \in \text{events}} \text{weight}_{\text{knn}(i)} \int \left|F_{\text{knn}(i)}(x) - F(x)\right|^p dF(x).$$

The knn approach suffers from a drawback: the impact of different events has very little connection with the weights, because some events are selected as nearest neighbours much more frequently than others. This effect can be suppressed by dividing the initial weight of the event by the number of times it is selected as a nearest neighbour.

A.5 Advantages and Disadvantages of Different Metrics

A.5.1 Theil and SDE

Let us compare two metrics that have proven most appropriate for our problem, SDE and Theil. We have some masses distributed uniformly in $[0,1]$, some constant α from interval $[.1,1]$. The predictions are correlated with mass via beta distribution. We have two distributions that are different in a way that they are symmetrical. SDE should show no changes if we flip the distribution, while the Theil should make difference between pit and peak. First distribution with a peak is obtained by generating a prediction for each event according to it mass:

$$p \sim \text{Beta}(\alpha\overline{m}, |m-\overline{m}|)$$

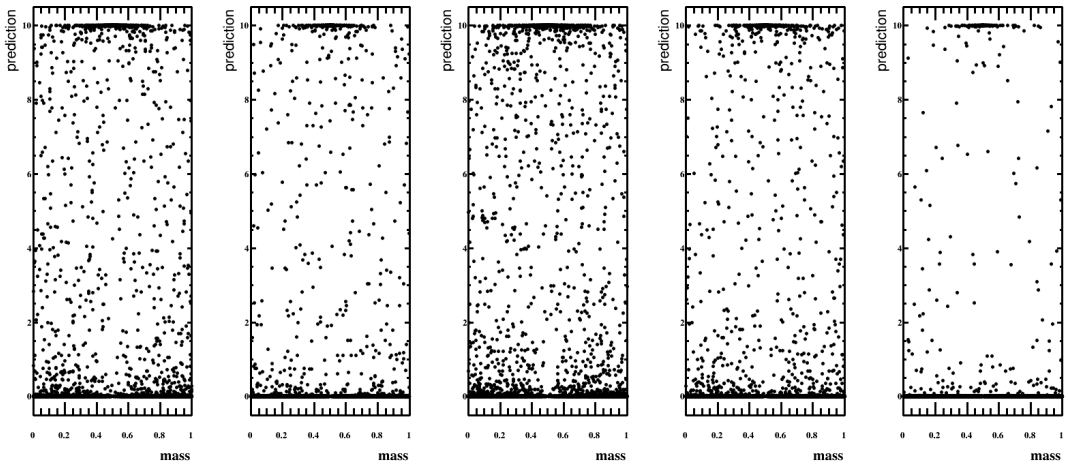
while the second one has minus sign in front. Figures 6 and 7 show the distribution of the predictions and classifier efficiency as a function of mass for the peak and pit distributions, respectively.

From these figures we can see that SDE has the same value and it is not able to make difference between these distributions. In the second case Theil has lower value which indicates that distribution is flatter. In the combination with SDE it can be used to detarmine the type of a distribution. Lower value of SDE can indicate that distribution is flat or has some narrow peaks or pits, and by using Theil we can distinguish between these two cases.

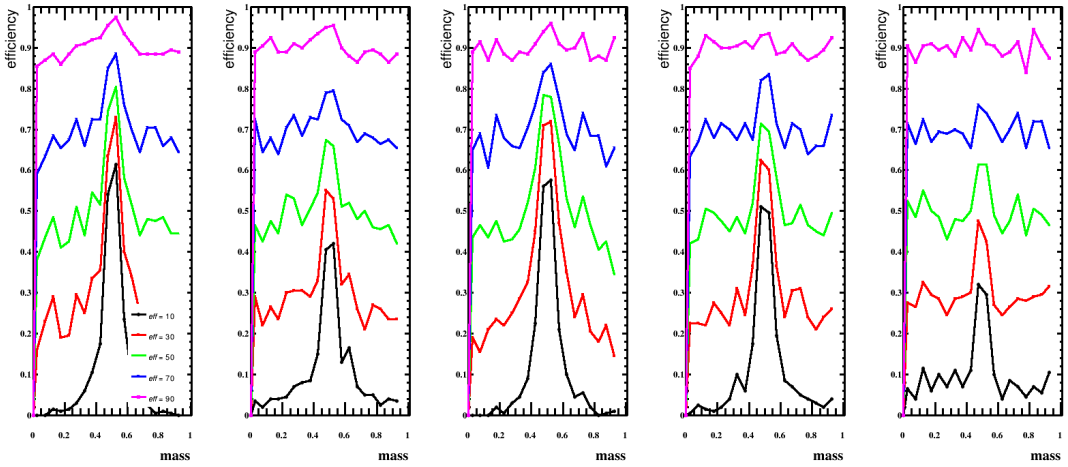
A.5.2 $D \to hhh$

When our classifiers where applied to data set $D \to hhh$ we got uniformity measures for the SDE and Theil metrics shown in Fig. 9.

Both metrics shown similar results, and that there is no significant difference on real data sets (as well as CvM). The SDE and Theil metrics can be used together in limit cases to more precisely determine nature of a distribution.

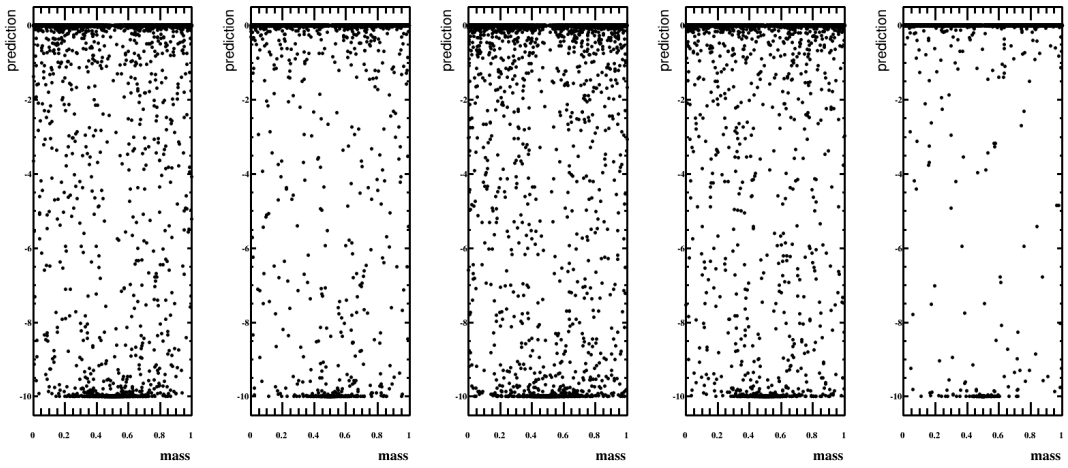


(a) Mass vs prediction.

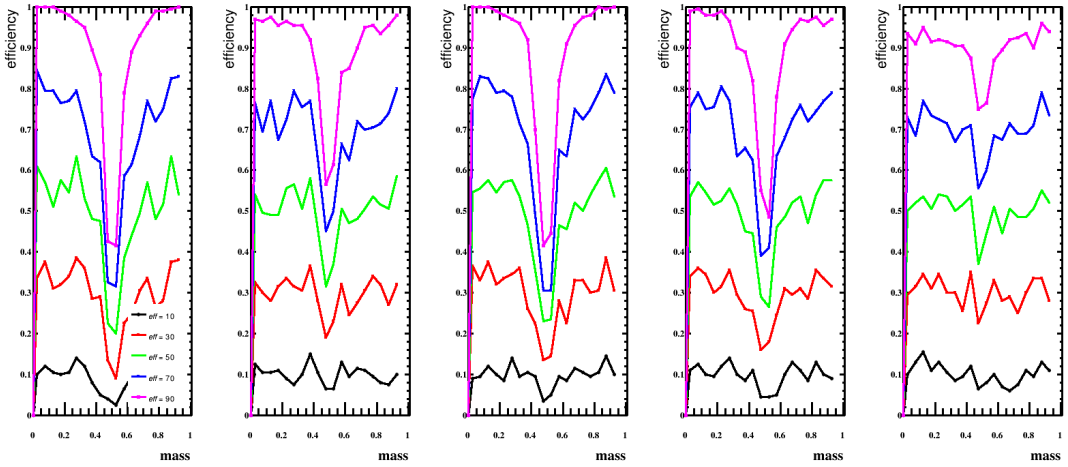


(b) Mass vs efficiency. The different coloured lines correspond to different global classifier efficiencies, as explained in the legend on the leftmost subplot.

Figure 6: Peak response distribution and efficiencies as a function of mass.



(a) Mass vs prediction.



(b) Mass vs efficiency. The different coloured lines correspond to different global classifier efficiencies, as explained in the legend on the leftmost subplot.

Figure 7: Pit response distribution and efficiencies as a function of mass.

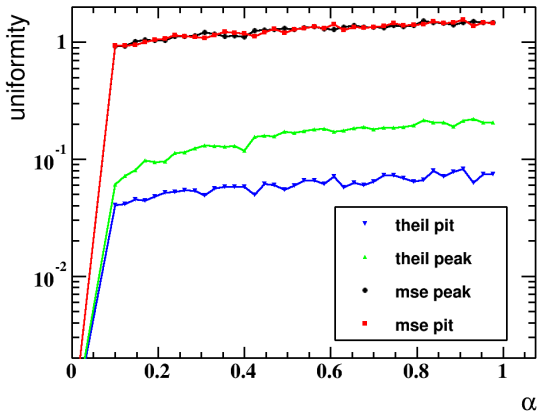
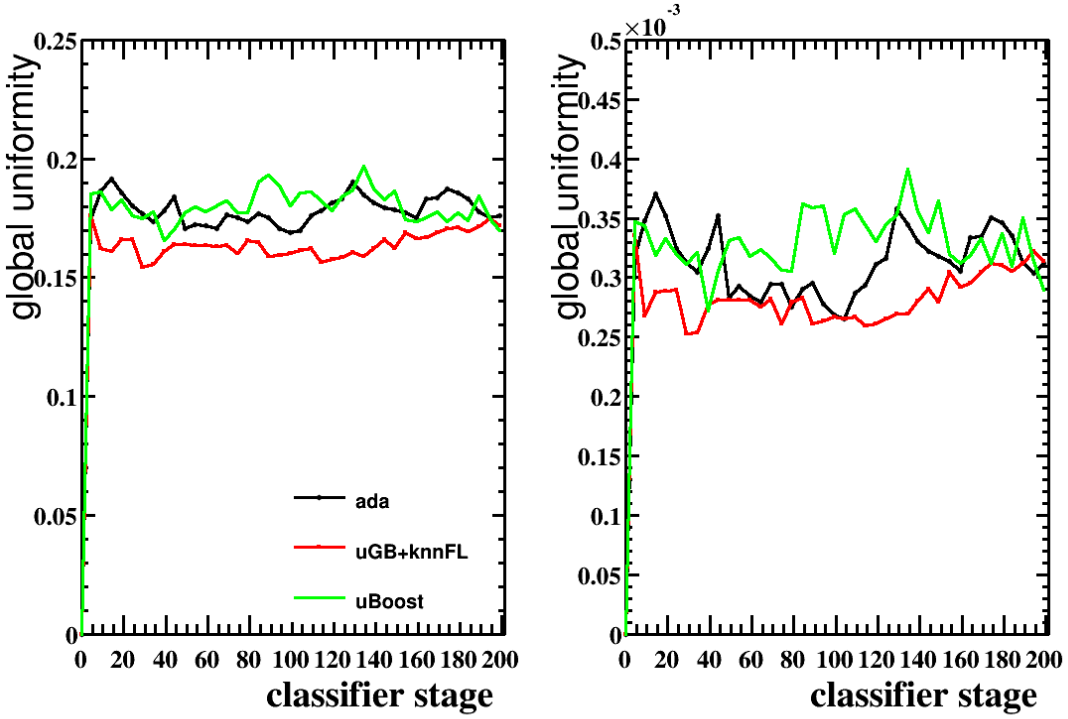
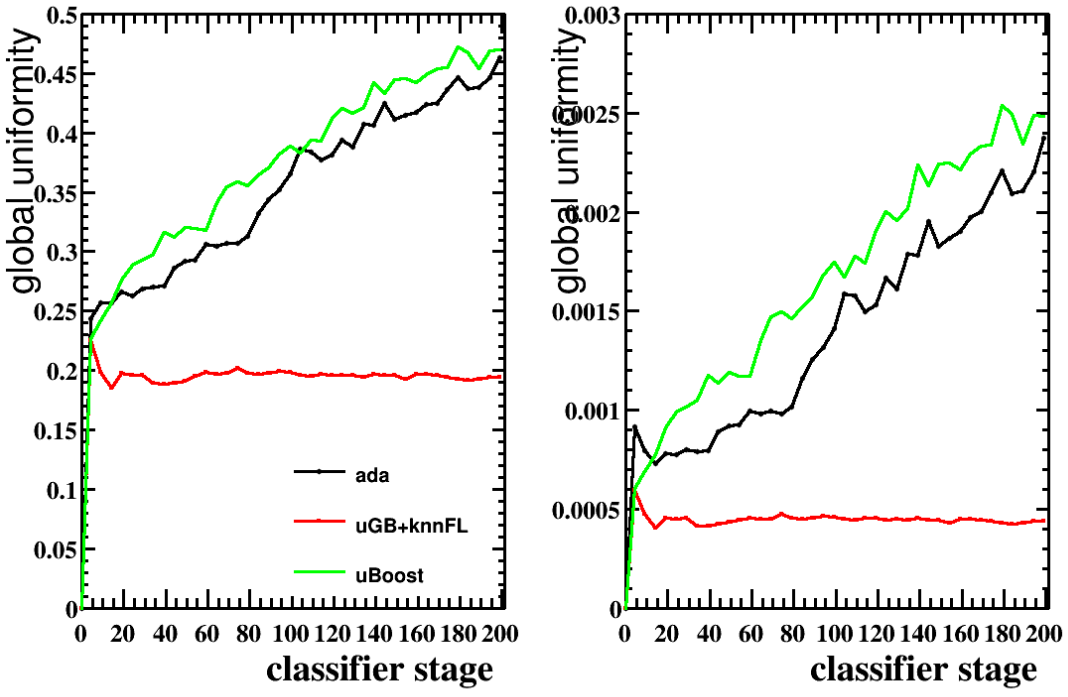


Figure 8: Comparison of SDE and Theil uniformity measures for different values of the constant α for the peak and pit distributions. The Theil can clearly distinguish between these two while the SDE measure cannot.



(a) Metrics for $D \to hhh$ signal.



(b) Metrics for $D \to hhh$ background.

Figure 9: Uniformity metrics for the $D \to hhh$ data set. The (top) signal and (bottom) background uniformities are plotted as a function of the training stage of a given classifier, listed in the legends on the leftmost plots.