Density Estimation Trees in High Energy Physics

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January 30th, 2015

Abstract
Density Estimation Trees can play an important role in exploratory data analysis for multi-dimensional, multi-modal data models of large samples. I briefly discuss the algorithm, a self-optimization technique based on kernel density estimation, and some applications in High Energy Physics.

1 Introduction
The usage of nonparametric density estimation techniques has seen a quick growth in the latest years both in High Energy Physics (HEP) and in other fields of Science dealing with multi-variate data samples. Indeed, the improvement in the computing resources available for data analysis allows today to process a much larger number of entries requiring more accurate statistical models. Avoiding parametrization for the distribution with respect to one or more variables allows to enhance accuracy removing unphysical constraints on the shape of the distribution. The improvement becomes more evident when considering the joint probability density function with respect to correlated variables, for whose model a too large number of parameters would be required.

Kernel Density Estimation (KDE) is a nonparametric density estimation technique based on the estimator

$$\hat{f}_{\text{KDE}}(x) = \frac{1}{N_{\text{tot}}} \sum_{i=1}^{N_{\text{tot}}} k(x - x_i),$$

where \(x = (x^{(1)}, x^{(2)}, ..., x^{(d)})\) is the vector of coordinates of the \(d\)-variate space \(S\) describing the data sample of \(N_{\text{tot}}\) entries. \(k\) is a normalized function referred to as kernel. KDE is widely used in HEP [Cranmer (2001); Poluektov (2014)] including notable applications to the Higgs boson mass measurement by the ATLAS Collaboration [Aad et al. (2014)]. The variables considered in the construction of the data-model are the mass of the Higgs boson candidate and the response of a Boosted Decision Tree (BDT) algorithm used to classify the data entries as Signal or Background candidates [Breiman et al. (1984)]. This solution allows to synthesize a set of variables, input of the
BDT, into a single variable, the BDT response, which is modeled. In principle, a multi-
variate data-model of the BDT-input variables may simplify the analysis and result into
a more powerful discrimination of signal and background. Though, the computational
cost of traditional nonparametric data-model (histograms, KDE, ...) for the sample
used for the training of the BDT, including $\mathcal{O}(10^6)$ entries, is prohibitive.

Data modelling, or density estimation, techniques based on decision trees are dis-
cussed in the literature of statistics and computer vision communities [Ram & Gray
(2011), Provost & Domingos (2000)], and with some optimization they are suitable for
HEP as they can contribute to solve both classification and analysis-automation prob-
lems in particular in the first, exploratory stages of data analysis.

In this paper I briefly describe the Density Estimation Tree (DET) algorithm, in-
cluding an innovative and fast cross-validation technique based on KDE and consider
few examples of successful usage of DETs in HEP.

2 The algorithm

A decision tree is an algorithm or a flowchart composed of internal nodes representing
tests of a variable or of a property. Nodes are connected to form branches, each ter-
mimates into a leaf, associated to a decision. Decision trees are extended to Density (or
Probability) Estimation Trees when the decisions are probability density estimations
of the underlying probability density function of the tested variables. Formally, the
estimator is written as

$$
\hat{f}(x) = \sum_{i=1}^{N_{\text{leaves}}} \frac{1}{N_{\text{tot}}} \frac{N(\text{leaf}_i)}{V(\text{leaf}_i)} I(x_i),
$$

(2)

where $N_{\text{leaves}}$ is the total number of leaves of the decision tree, $N(\text{leaf}_i)$ the number
of entries associated to the $i$-th leaf, and $V(\text{leaf}_i)$ is its volume. If a generic data entry,
deefined by the input variables $x$, would fall within the $i$-th leaf, then $x$ is said to be in
the $i$-th leaf, and the characteristic function of the $i$-th leaf,

$$
I(x) = \begin{cases} 
1 & \text{if } x \in \text{leaf}_i \\
0 & \text{if } x \notin \text{leaf}_i
\end{cases},
$$

(3)

equals unity. By construction, all the characteristic functions associated to the other
leaves, are null. Namely,

$$
x \in \text{leaf}_i \Rightarrow x \notin \text{leaf}_j \quad \forall j : j \neq i.
$$

(4)

The training of the Density Estimation Tree is divided in three steps: tree growth,
pruning, and cross-validation. Once the tree is trained it can be evaluated using the
simple estimator of Equation (2) or some evolution obtained through smearing or inter-
polation. These steps are briefly discussed below.
2.1 Tree growth

As for other decision trees, the tree growth is based on the minimization of an estimator of the error. For DETs, the error is the Integrated Squared Error (ISE), defined as

$$R = \text{ISE}(f, \hat{f}) = \int_S (\hat{f}(x) - f(x))^2 \, dx.$$  \hfill (5)

It can be shown (see for example [Anderlini 2015] for a pedagogical discussion) that, for large samples, the minimization of the ISE is equivalent to the minimization of

$$R_{\text{simple}} = -\sum_{i=1}^{N_{\text{leaves}}} \left( \frac{N(\text{leaf}_i)}{N_{\text{tot}}} \right)^2 \frac{1}{V(\text{leaf}_i)}.$$  \hfill (6)

The tree is therefore grown by defining the replacement error

$$R(\text{leaf}_i) = -\frac{(N(\text{leaf}_i))^2}{N_{\text{tot}}^2 V(\text{leaf}_i)},$$  \hfill (7)

and iteratively splitting each leaf $\ell$ to two sub-leaves $\ell_L$ and $\ell_R$ maximising the residual gain

$$G(\ell) = R(\ell) - R(\ell_L) - R(\ell_R).$$  \hfill (8)

The growth is arrested, and the splitting avoided, when some stop condition is matched. The most common stop condition is $N(\ell_L) < N_{\min}$ or $N(\ell_R) < N_{\min}$, but it can be OR-ed with some alternative requirement, for example on the widths of the leaves.

A more complex stop condition is obtained by defining a minimal leaf-width $l^{(m)}$ with respect to each dimension $m$. Splitting by testing $x^{(m)}$ is forbidden if the width of one of the resulting leaves is smaller than $l^{(m)}$. When no splitting is allowed the branch growth is stopped. This stop condition requires to issue the algorithm with a few more input parameters, the leaf-width thresholds, but is very powerful against over-training. Besides, the determination of reasonable leaf-widths is an easy task for most problems, once the expected resolution on each variable is known.

Figure 1 depicts a simple example of the training procedure on a two-dimensional real data-sample.

2.2 Tree pruning

DETs can be overtrained. Overtraining (or overfitting) occurs when the statistical model obtained through the DET describes random noise or fluctuations instead of the underlying distribution. The effect results in trees with isolated leaves with small volume and therefore associated to large density estimations, surrounded by almost-empty leaves. Overtraining can be reduced through pruning, an a posteriori processing of the tree structure. The basic idea is to sort the nodes in terms of the actual improvement they introduce in the statistical description of the data model. Following a procedure common for classification and regression trees, the regularized error is defined as

$$R_\alpha(\text{node}_i) = \sum_{j \in \text{leaves of node}_i} R(\text{leaf}_j) + \alpha C(\text{node}_i),$$  \hfill (9)
where $\alpha$ is named *regularization parameter*, and the index $j$ runs over the sub-nodes of $\text{node}_i$, with no further sub-nodes (its leaves). \( C(\text{node}_i) \) is the *complexity function* of leaf \( i \).

Several choices for the complexity function are possible. In the literature of classification and regression trees, a common definition is to set \( C(\text{node}_i) \) to the number of terminal nodes (or leaves) attached to $\text{node}_i$. Such a complexity function provides a top-down simplification technique which is complementary to the stop condition. Unfortunately, in practice, the optimization through the pruning obtained with a number-of-leaves complexity function is ineffective against overtraining, if the stop condition is suboptimal.

An alternative cost function, based on the depth of the node in the tree development, provides a bottom-up pruning, which can be seen as an *a posteriori* optimization of the stop condition.

An example of the two cost functions discussed is shown in Figure 1.

If \( R_{\alpha}(\text{node}_i) > R(\text{node}_i) \) the splitting of the $i$-th node is pruned, and its sub-nodes merged into a unique leaf. Each node is therefore associated to a threshold value...
of the regularization parameter, so that if $\alpha$ is larger than the threshold $\alpha_i$, then the $i$-th node is pruned. Namely,

$$\alpha_i = \frac{1}{C(\text{node}_i)} \left( R(\text{node}_i) - \sum_{j \in \text{leaves of node}_i} R(\text{leaf}_j) \right).$$

(10)

The quality of the estimator $Q(\alpha)$, defined and discussed below, can then be evaluated per each threshold value of the regularization parameter. The optimal pruning is obtained for

$$\alpha = \alpha_{\text{best}} : \quad Q(\alpha_{\text{best}}) = \max_{\alpha \in \{\alpha_i\}} Q(\alpha).$$

(11)

### 2.3 Cross-validation

The determination of the optimal regularization parameter is named cross-validation, and many different techniques are possible, depending on the choice of the quality function.

A common cross-validation technique for classification and regression trees is the Leave-One-Out (LOO) cross-validation and consists in the estimation of the underlying probability distribution through a resampling of the original dataset. For each data entry $i$, a sample containing all the entries but $i$ is used to train a DET. The ISE is redefined as

$$R_{\text{LOO}}(\alpha) = \int_{\mathcal{S}} \left( \hat{f}^\alpha(x) \right)^2 \, dx - \frac{2}{N_{\text{tot}}} \sum_{i=1}^{N_{\text{tot}}} \hat{f}_{\text{not}}^\alpha i(x_i),$$

(12)

where $\hat{f}^\alpha(x)$ is the probability density estimation obtained with a tree pruned with regularization parameter $\alpha$, and $\hat{f}_{\text{not}}^\alpha i(x)$ is the analogous estimator obtained from a dataset obtained removing the $i$-th entry from the original sample. The quality function is

$$Q(\alpha) = -R_{\text{LOO}}(\alpha).$$

(13)

The application of the LOO cross-validation is very slow and requires to build one decision tree per entry. When considering the application of DETs to large samples, containing for example one million of entries, the construction of a million of decision trees and their evaluation per one million of threshold regularization constants becomes unreasonable.

A much faster cross-validation is obtained comparing the estimation obtained with the DET with a triangular-kernel density estimation

$$f_k(x) = \frac{1}{N_{\text{tot}}} \times$$

$$\times \sum_{i=1}^{N_{\text{tot}}} \prod_{k=1}^{d} \left( 1 - \left| \frac{x - x_i}{h_k} \right| \right) \theta \left( 1 - \left| \frac{x - x_i}{h_k} \right| \right),$$

(14)

where $\theta(x)$ is the Heaviside step function, $k$ runs over the $d$ dimensions of the coordinate space $\mathcal{S}$, and $h_k$ is the kernel bandwidth with respect to the variable $x^{(k)}$. 

5
The quality function is

$$Q^{ker}(\alpha) = -\int_S (f_\alpha(x)^2 - f_k(x)^2)^2 \, dx.$$  \hfill (15)

The choice of a triangular kernel allows to analytically solve the integral writing that

$$Q^{ker}(\alpha) = \frac{1}{N_{tot}^2} \sum_{j=1}^{N_{leaves}} \frac{N(\text{leaf}_j^\alpha)}{V(\text{leaf}_j^\alpha)} (2N_j - N(\text{leaf}_j^\alpha)) + \text{const},$$  \hfill (16)

where \(\text{leaf}_j^\alpha\) represents the \(j\)-th leaf of the DET pruned with regularization constant \(\alpha\), and

$$N_j = \sum_{i=1}^{N_{tot}} \sum_{k=1}^d x_{jk}(x_i; h_k) = \sum_{i=1}^{N_{tot}} \sum_{k=1}^d \left[ u_{ij}^{(k)} - \ell_{ij}^{(k)} + \frac{(u_{ij}^{(k)} - x_i^{(k)})^2}{2h_k} \text{sign} \left( u_{ij}^{(k)} - x_i^{(k)} \right) + \frac{(\ell_{ij}^{(k)} - x_i^{(k)})^2}{2h_k} \text{sign} \left( x_i^{(k)} - \ell_{ij}^{(k)} \right) \right].$$  \hfill (17)

with \(\text{sign}(x) = 2\theta(x) - 1\), and

$$\begin{cases} u_{ij}^{(k)} &= \min \left( x_{\text{max}}^{(k)}(\text{leaf}_j^\alpha), x_i^{(k)} + h_k \right) \\ \ell_{ij}^{(k)} &= \max \left( x_{\text{min}}^{(k)}(\text{leaf}_j^\alpha), x_i^{(k)} - h_k \right). \end{cases}$$  \hfill (18)

In Equation 18, \(x_{\text{max}}^{(k)}(\text{leaf}_j^\alpha)\) and \(x_{\text{min}}^{(k)}(\text{leaf}_j^\alpha)\) represent the upper and lower boundaries of the \(j\)-th leaf, respectively.

An interesting aspect of this technique is that a large part of the computational cost is hidden in the definition of \(N_j\) which does not depend on \(\alpha\), and therefore can be calculated only once per node, \textit{de facto} reducing the computational complexity by a factor \(N_{tot} \times N_{leaves}\).

### 2.4 DET Evaluation: smearing and interpolation

One of the major limitations of DETs is the existence of sharp boundaries which are unphysical. Besides, a small variation of the position of a boundary can lead to a large variation in the final result, when using DETs for data modelling. Two families of solutions are discussed here: smearing and linear interpolation. The former can be seen as a convolution of the density estimator with a resolution function. The effect is that sharp boundaries disappear and residual overtraining is cured, but as long as the resolution function has a fixed width, the adaptability of the DET algorithms is partially lost: resolution will never be smaller than the smearing function width.

An alternative technique is interpolation, assuming some behaviour (usually linear) of the density estimator between the middle points of each leaf. The density estimation
at the center of each leaf is assumed to be accurate, therefore overtraining is not cured, and may lead to catastrophic density estimations. Interpolation is treated here only marginally. It is not very robust, and it is hardly scalable to more than two dimensions. Still, it may represent a useful smoothing tool for samples composed of contributions with resolutions spanning a large interval, for which adaptability is crucial.

2.4.1 Smearing

The smeared version of the density estimator can be written as

\[
\hat{f}_s(x) = \int_S \hat{f}(z) w \left( \frac{x - z}{h_k} \right) dx,
\]

where \( w(x) \) is the resolution function. Using a triangular resolution function \( w(t) = (1 - |t|) \theta(1 - |t|) \),

\[
\hat{f}_s(x) = \frac{N_{\text{leaves}}}{d} \prod_{k=1}^{d} I_{jk}(x; h_k),
\]

where \( I_{jk}(x; h_k) \) was defined in Equation 17.

Note that the evaluation of the estimator does not require a loop on the entries, factorized within \( I_{jk} \).

2.4.2 Interpolation

As mentioned above, the discussion of interpolation is restrained to two-dimensional problems. The basic idea of linear interpolation is to associate each \( x \in S \) to the three leaf centers defining the smallest triangle inscribing \( x \) (step named padding or tessellation). Using the positions of the leaf centers, and the corresponding values of the density estimator as coordinates, it is possible to define a unique plane. The plane can then be “read” associating to each \( x \in S \) a different density estimation. The key aspect of the algorithm is padding. Padding techniques are discussed for example in de Berg et al. (2008). The algorithm used in the examples below is based on Delaunay tessellation as implemented in the ROOT libraries Brun & Rademakers (1997). Extensions to more than two dimensions are possible, but non trivial and computationally expensive. Instead of triangles, one should consider hyper-volumes defined by \((d + 1)\) leaf centers, where \( d \) is the number of dimensions. Moving to parabolic interpolation is also reasonable, but the tessellation problem for \((d + 2)\) volumes is less treated in the literature, requiring further development.

3 Timing and computational cost

The discussion of the performance of the algorithm is based on an single-core C++ implementation. Many-core tree growth, with each core growing an independent branch, is an embarrassing parallel problem. Parallelization of the cross-validation is also possible, if each core tests the Quality function for a different value of the regularization
Figure 3: CPU time to train and evaluate a self-optimized decision tree as a function of the number of entries \( N_{\text{tot}} \). On the top, a stop criterion including a reasonable leaf-width threshold is used; on the bottom it is replaced with a very loose threshold. The time needed to train a Kernel Density Estimation (KDE) is also reported for comparison.

Parameter \( \alpha \). ROOT libraries are used to handle the input-output, but the algorithm is independent, relying on STL containers for data structures.

The advantage of DET algorithms over kernel-based density estimators is the speed of training and evaluation. The complexity of the algorithm is \( N_{\text{leaves}} \times N_{\text{tot}} \). In common use cases, the two quantities are not independent, because for larger samples it is reasonable to adopt a finer binning in particular in the tails. Therefore, depending on the stop condition the computational cost scales with the size of the data sample as \( N_{\text{tot}} \) to \( N_{\text{tot}}^2 \). Kernel density estimation in the ROOT implementation is found to scale as \( N_{\text{tot}}^2 \).

Reading time scales roughly as \( N_{\text{leaves}} \).

Figure 3 reports the comparison of the CPU time needed to train, optimize and sample on a \( 200 \times 200 \) grid a DET; the time to train a kernel density estimation on the same sample is also reported. The two plots show the results obtained with reasonable and loose stop conditions based on the minimal leaf width. It is interesting to observe that when using a loose leaf-width condition, \( N_{\text{leaves}} \propto N_{\text{tot}} \) and the algorithm scales as \( N_{\text{tot}}^2 \). Increasing the size of the sample, the leaf-width condition becomes relevant and the computational cost of the DET deflects from \( N_{\text{tot}}^2 \), and starts being convenient with respect to KDE.

4 Applications in HEP

In this section I discuss a few possible use cases of density estimation trees in High Energy Physics. In general, the technique is applicable to all problems involving data modeling, including efficiency determination and background subtraction. However, for these applications KDE is usually preferable, and only in case of too large samples, in some development phase of the analysis code, it may be reasonable to adopt DET instead. Here I consider applications where the nature of the estimator, providing fast training and fast integration, introduces multivariate density estimation into problems traditionally treated alternatively. The examples are based on a dataset of real data collected during the \( pp \) collision programme of the Large Hadron Collider at CERN by the LHCb experiment. The dataset has been released by the LHCb Collaboration in the
framework of the LHCb Masterclass programme. The detail of the reconstruction and selection, not relevant to the discussion of the DET algorithm, are discussed in Ref. [LHCb Collaboration (2014)]. The data sample contains combinations of a pion ($\pi$) and a kaon ($K$), two light mesons, loosely consistent with the decay of a $D^0$ meson.

Figure 4 shows the invariant mass of the $K\pi$ combination, i.e. the mass of a hypothetical mother particle decayed to the reconstructed kaon and pion. Two contributions are evident: a peak due to real $D^0$ decays, with the invariant mass which is consistent with the mass of the $D^0$ meson, and a flat contribution due to the random combination of kaons and pions, with an invariant mass which is a random number. The peaked contribution is named “Signal”, the flat one is the “Background”.

An important aspect of data analysis in HEP consists in the disentanglement of different contributions to allow statistical studies of the signal without pollution from background. In next two Sections, I consider two different approaches to signal-background separation. First, an application of DETs to the optimization of the rectangular selection is discussed. Then, a more powerful statistical approach based on likelihood analysis is described.

### 4.1 Selection optimization

When trying to select a relatively pure sample of signal candidates, rejecting background, it is important to define an optimal selection strategy based on the variables associated to each candidate. For example, a large momentum of the $D^0$ candidate ($D^0 p_T$) is more common for signal than for background candidates, therefore $D^0$ candidates with a $p_T$ below a certain threshold can be safely rejected. The same strategy can be applied to the transverse momentum of the kaon and of the pion separately, which are obviously correlated with the momentum of their mother candidate, the $D^0$ meson. Another useful variable is some measure of the consistency of the reconstructed flight direction of the $D^0$ candidate with its expected origin (the $pp$ vertex). Random combinations of a pion and a kaon are likely to produce $D^0$ candidates poorly aligned
with the point where \( D^0 \) are expected to be produced. In the following I will use the Impact Parameter (IP) defined as the distance between the reconstructed flight direction of the \( D^0 \) meson and the \( pp \) vertex.

The choice of the thresholds used to reject background to enhance signal purity often relies on simulated samples of signal candidates, and on data regions which are expected to be well dominated by background candidates. In the example discussed here, the background sample is obtained selecting the \( D^0 \) candidates with a mass \( 1.815 < m(D^0) < 1.840 \text{ GeV}/c^2 \) or \( 1.890 < m(D^0) < 1.915 \text{ GeV}/c^2 \).

The usual technique to optimize the selection is to count the number of simulated signal candidates \( N_S \) and background candidates \( N_B \) surviving a given combination of thresholds \( t \), and picking the combination which maximizes some metric \( M \), for example

\[
M(t) = \frac{S(t)}{S(t) + B(t) + 1} = \frac{\epsilon_S N_S(t)}{\epsilon_S N_S(t) + \epsilon_B N_B(t) + 1} \tag{21}
\]

where \( \epsilon_S (\epsilon_B) \) is the normalization factors between the number of entries \( N_{S}^{\infty} (N_{B}^{\infty}) \) in the pure sample and the expected yields \( S^{\infty} (B^{\infty}) \) in the mixed sample prior the selection.

When the number of thresholds to be optimized is large, the optimization may require many iterations. Only in absence of correlation between the variables used in the selection, the optimization can be factorized reducing the number of iterations. For large samples, counting the surviving candidates at each iteration may become very expensive.

Two DET estimators \( \hat{f}_S(x) \) and \( \hat{f}_B(x) \) for the pure samples can be used to reduce the computational cost of the optimization from \( N_{\text{tot}} \) to \( N_{\text{leaves}} \), integrating the distribution leaf by leaf instead of counting the entries.

The integral of the density estimator in the rectangular selection \( R \) can be formally written as

\[
\int_R \hat{f}(x)dx = \frac{1}{N_{\text{tot}}} \sum_{i=1}^{N_{\text{leaves}}} \frac{V(\text{leaf}_i \cap R)}{V(\text{leaf}_i)} N(\text{leaf}_i). \tag{22}
\]

The optimization requires to find

\[
R = R_{\text{opt}} : \quad M_I(R_{\text{opt}}) = \max_{R \subset S} M_I(R), \tag{23}
\]

with

\[
M_I(R) = \frac{\int_R \hat{f}_S(x)dx}{1 + \int_R \hat{f}_S(x)dx + B^{\infty} \int_R \hat{f}_B(x)dx}. \tag{24}
\]

Figure 5 reports a projection of \( \hat{f}_S \) and \( \hat{f}_B \) onto the plane defined by the impact parameter (IP) and the proper decay time of the \( D^0 \) meson. The two variables are obviously correlated, because \( D^0 \) candidates poorly consistent with their expected origin are associated to a larger decay time in the reconstruction procedure, which is based on the measurements of the \( D^0 \) flight distance and of its momentum. The estimation reproduces correctly the correlation, allowing better background rejection combining the discriminating power of the two variables when defining the selection criterion.
Figure 5: Density Estimation of pure signal (top) and pure background (bottom) samples, projected onto the plane of the impact parameter and proper decay time. The entries of the data sample are shown as black dots superposed to the color scale representing the density estimation.

4.2 Likelihood analyses

Instead of an optimization of the rectangular selection it is reasonable to separate signal and background using multivariate techniques as Classification Trees or Neural Networks.

A multivariate statistic based on likelihood can be built using DETs:

$$\Delta \log \mathcal{L}(x) = \log \frac{\hat{f}_S(x)}{\hat{f}_B(x)}.$$  \hspace{1cm} (25)

The advantage of using density estimators over Classification Trees is that likelihood functions from different samples can be easily combined. Consider the sample of $K\pi$ combinations described above. Among the variables defined to describe each candidate there are Particle Identification (PID) variables, response of an Artificial Neural Network (ANN) trained on simulation, designed to provide discrimination, for example, between kaons and pions. The distributions of PID variables are very difficult to simulate properly because the conditions of the detectors used for PID are not perfectly stable during the data acquisition. It is therefore preferred to use pure samples of real kaons and pions to study the distributions instead of simulating them. The distributions obtained depends on the particle momentum $p$, and on the angle $\theta$ between the particle momentum and the proton beams. These variables are obviously correlated to the transverse momentum which, as discussed in the previous section, is a powerful discriminating variable, whose distribution has to be taken from simulation, and is in general different from simulated samples. To shorten the equations, below I apply the technique to the kaon only, but the same could be done for the identification of the pion. The multivariate statistic can therefore be rewritten as

$$\Delta \log \mathcal{L}(p_T(D^0), IP, p_T(K), p_T(\pi), p_K, \theta_K, PID K_K) =$$

$$\frac{\hat{f}_S(p_T(D^0), IP, p_T(K), p_T(\pi))}{\hat{f}_B(p_T(D^0), IP, p_T(K), p_T(K), PID K_K)} \times$$

$$\frac{\hat{f}_K(PID K_K, p_K, \theta_K)}{\int \hat{f}_K(PID K_K, p_K, \theta_K) d(PID K_K)},$$  \hspace{1cm} (26)
where \( \text{PID} K_K \) is the response of the PID ANN for the kaon candidate and the kaon hypothesis, and \( f_K \) is the DET model built from a pure calibration sample of kaons.

The opportunity of operating this disentanglement is due to the properties of the probability distribution functions which are not trivially transferable to Classification Trees. Note that, as opposed to the previous use case, where integration discourages smearing because Equation 22 is not applicable to the smeared version of the density estimator, likelihood analyses can benefit of smearing techniques for the evaluation of the first term in Equation 26 while for the second term, smearing can be avoided thanks to the large statistics usually available for calibration samples.

5 Conclusion

Density Estimation Trees are fast and robust algorithm providing probability density estimators based on decision trees. They can be grown cheaply beyond overtraining, and then pruned through a kernel-based cross-validation. The procedure is computationally cheaper than pure kernel density estimation because the evaluation of the latter is performed only once per leaf.

Integration and projections of the density estimator are also fast, providing an efficient tool for many-variable problems involving large samples.

Smoothing techniques discussed here include smearing and linear interpolation. The former is useful to fight overtraining, but challenges the adaptability of the DET algorithms. Linear interpolation requires tessellation algorithms which are nowadays available for problems with three or less variables, only.

A few applications to high energy physics have been illustrated using the \( D^0 \to K^- \pi^+ \) decay mode, made public by the LHCb Collaboration in the framework of the Masterclass programme. Selection optimization and likelihood analyses can benefit of different features of the Density Estimation Tree algorithms. Optimization problems require fast integration of a many-variable density estimator, made possible by its simple structure with leaves associated to constant values. Likelihood analyses benefit of the speed of the method which allows to model large calibration samples in a time much reduced with respect to KDE, and offering an accuracy of the statistical model much better than histograms.

In conclusion, Density Estimation Trees are interesting algorithms which can play an important role in exploratory data analysis in the field of High Energy Physics, filling a gap between the simple histograms and the expensive Kernel Density Estimation, and becoming more and more relevant in the age of the Big Data samples.

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