Predicting Physics Observables by Analysing LHC-like Data: From ROOT Structures to Machine Learning

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Abstract

This document serves as a structured technical report for the project "Predicting Physics Observables by Analysing LHC-like Data." The study documents the end-to-step exploration of ROOT files, the understanding of high-energy physics data structures, and the application of machine learning techniques to classify heavy-flavor decay topologies. We distinguish between aggregated analysis outputs and event-wise `TTree` structures, establishing the necessity of columnar data for predictive modeling.

The analysis focuses on the reconstruction of D^{*+} mesons via the $D^0\pi^+$ decay channel. By defining topological variables—such as pointing angles and impact parameters—in the $3.67 < p_T < 5.67$ GeV/c interval, we separate signal from combinatorial background. The report demonstrates that while topological variables alone provide strong discrimination (BDT AUC ≈ 0.94), the incorporation of Particle Identification (PID) variables into a Neural Network architecture further enhances classification performance, achieving an accuracy of 84.14%.

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1 Introduction

High-energy physics experiments, such as those conducted at the Large Hadron Collider (LHC), generate extremely large and structured datasets. These datasets are commonly stored using the ROOT framework, which provides efficient data storage, access, and visualization capabilities. The primary objective of this project is to develop a systematic understanding of these files and their internal structures as a first step toward predicting physics observables. This report documents the workflow from raw data inspection to the definition of physics-motivated features suitable for training machine learning classifiers.

2 Understanding ROOT Data Structures

A fundamental prerequisite for this analysis is distinguishing between different storage formats within the ROOT ecosystem. We analyzed two distinct file types to determine their suitability for machine learning.

2.1 Analysis of Aggregated Outputs

The file `AnalysisResults67.root` was inspected to understand standard analysis outputs. Using the ROOT command 'f->ls()', it was observed that the file is organized into task-based directories such as `track-propagation` and `hf-task-dstar-to-d0-pi`.

Detailed inspection using the Python 'uproot' library revealed that these directories contain exclusively histogram objects (`TH1F`, `TH2F`).

```
1 import uproot
2 file = uproot.open("AnalysisResults67.root")
3 # Output confirms histogram-only nature
4 # hDCAxyVsPtRec;1 -> TH2F
```

Listing 1: Python inspection of ROOT objects

Because histograms represent aggregated statistical summaries rather than per-event records, this format was deemed unsuitable for event-level predictive modeling.

2.2 Event-Wise Data Structures (TTrees)

For machine learning applications, we utilized the file `Prompt_DstarToD0Pi.root`. Unlike the analysis results, this file contains a top-level `TTree` object named `treeMLDstar`.

2.2.1 Concept of a TTree

A `TTree` functions as a columnar database where each row represents a candidate (an entry) and each column represents a variable (a branch). The specific tree analyzed contains 1,040,228 entries. Crucially, the branches store scalar values (Single Precision Float `/F` or Boolean `/B`), making the structure "flat" and ideal for conversion into tabular formats like pandas DataFrames.

2.2.2 Python Integration

Using 'uproot', the tree was converted to a DataFrame with shape $(1040228, 51)$, confirming the availability of 51 distinct features per candidate for analysis.

3 Fundamental Particle Physics Background

3.1 Relativistic Kinematics

At LHC energies, particle velocities approach the speed of light ($v \approx c$), necessitating the use of Special Relativity. The dynamics are described by four-vectors $p^\mu = (E, \vec{p})$, satisfying the invariant relation:

$$E^2 = p^2c^2 + m^2c^4 \tag{1}$$

In this analysis, we employ **Natural Units** ($\hbar = c = 1$), simplifying the relation to $E^2 = p^2 + m^2$, where energy, momentum, and mass are expressed in GeV.

3.2 Coordinate Systems

To account for collider geometry, we utilize Lorentz-invariant coordinates:

- **Rapidity (y):** A measure of relativistic velocity that is additive under Lorentz boosts.
- **Pseudorapidity (η):** An approximation for massless particles defined as $\eta = -\ln(\tan(\theta/2))$.
- **Transverse Momentum (p_T):** Defined as $p_T = \sqrt{p_x^2 + p_y^2}$. This component is perpendicular to the beam axis and invariant under longitudinal boosts.

3.3 Heavy-Flavor Physics

The analysis focuses on heavy-flavor mesons containing Charm (c) or Bottom (b) quarks. These quarks are produced in initial hard scattering processes and serve as probes for Quantum Chromodynamics (QCD) and the Quark-Gluon Plasma (QGP). We distinguish between two production mechanisms:

1. **Prompt:** Produced directly at the primary vertex from charm hadronization.
2. **Non-Prompt:** Originating from the weak decay of long-lived B mesons ($B \to D^{*+} + X$), characterized by displaced vertices.

4 Experimental Reconstruction of D Mesons

4.1 Decay Channels

The D^{*+} meson is reconstructed via the "Golden Channel":

$$D^{*+} \to D^0 \pi^+_{soft} \to (K^- \pi^+)\pi^+_{soft} \tag{2}$$

The "soft" pion has very low momentum due to the small mass difference between the D^{*+} and D^0, providing a unique kinematic signature that suppresses background.

4.2 Transverse Momentum Binning

The analysis is performed in differential bins of transverse momentum (p_T). This is physically motivated by the power-law nature of particle production ($dN/dp_T \propto p_T^{-n}$). Furthermore, decay topology is highly p_T-dependent; higher momentum particles are more Lorentz boosted ($\gamma = E/m$), resulting in longer flight distances ($L \approx \beta\gamma c\tau$).

To avoid biasing the machine learning model with kinematic correlations, we perform the classification in specific intervals. For this report, we focus on the representative interval:

$$\mathbf{3.67 < p_T < 5.67\ GeV/c} \tag{3}$$

This range offers a balance between statistical precision and topological separation power.

5 Exploratory Analysis of Topological Variables

Before training classifiers, we validated the discriminating power of topological variables using the Prompt, Non-Prompt, and Background datasets. All distributions analyzed below are normalized to unit area to compare shapes.

5.1 Cosine of Pointing Angle ($cos\theta_p$)

The pointing angle measures the alignment between the D^0 momentum vector $\vec{p}$ and the displacement vector $\vec{L}$ connecting the primary and secondary vertices:

$$\cos\theta_p = \frac{\vec{L} \cdot \vec{p}}{|\vec{L}||\vec{p}|} \tag{4}$$

Signal candidates (Prompt and Non-Prompt) exhibit values near 1.0 due to momentum conservation, whereas background candidates show a broader distribution. This variable is the primary discriminator against combinatorial background.

5.2 Transverse Decay Length (L_{xy})

Defined as the distance the D^0 travels in the transverse plane ($L_{xy} = |\vec{r}_{SV} - \vec{r}_{PV}|_{xy}$). Prompt candidates peak at zero, while Non-Prompt candidates exhibit a significant tail due to the finite lifetime of the parent B meson.

5.3 Impact Parameter Product

Defined as the product of the impact parameters of the two D^0 daughter tracks (K, π). Signal candidates typically have specific sign correlations resulting from a common displaced vertex, distinct from the random distribution of the background.

5.4 Soft Pion Impact Parameter

Although the soft pion originates effectively at the D^{*+} production point, its impact parameter relative to the primary vertex is sensitive to the production mechanism:

- **Prompt:** D^{*+} produced at PV $\rightarrow$ small IP.
- **Non-Prompt:** D^{*+} produced at displaced B-vertex $\rightarrow$ larger IP distribution.

The EDA confirms that this variable separates prompt from non-prompt signals effectively.

Having established the physical validity of these topological features, the next stage of the analysis quantifies their inter-dependencies through correlation matrices before implementing multivariate classifiers.

6 Correlation Analysis of Input Variables

Before proceeding to multivariate training, it is essential to quantify the statistical dependencies among the selected topological variables. A classifier, such as a Boosted Decision Tree (BDT) or Neural Network, performs optimally when input features provide complementary information.

6.1 Pearson Correlation Matrix

We constructed a correlation matrix using the Pearson coefficient, $\rho_{xy} = \frac{\mathrm{cov}(x,y)}{\sigma_x \sigma_y}$, evaluated on candidates within the $3.67 < p_T < 5.67$ GeV/c interval.

6.2 Physical Interpretation

The analysis revealed the following structural dependencies:

- **Pointing Angles (Strong Correlation):** The strongest correlation was observed between the 3D pointing angle (`fCpaD0`) and the transverse pointing angle (`fCpaXYD0`). This is physically expected, as both variables measure the alignment of the momentum vector with the decay vertex displacement; the latter is simply a projection of the former onto the transverse plane.
- **Independence of Decay Length:** The transverse decay length (`fDecayLengthXYD0`) showed relatively weak correlations with the impact parameter variables. This suggests that the distance traveled by the meson provides independent discrimination power compared to the geometric pointing accuracy.

Implication for Training: Despite the correlation between pointing angles, both were retained for the analysis. Machine learning models can often exploit subtle differences between projected and 3D variables to correct for detector resolution effects.

7 Baseline Classification: Boosted Decision Trees

To establish a performance baseline, a Boosted Decision Tree (BDT) was trained using only the topological variables described in the previous section. The classifier outputs a continuous score $s \in$, representing the probability of a candidate being a prompt signal.

7.1 Performance Evaluation (ROC Analysis)

We evaluated the separation power using Receiver Operating Characteristic (ROC) curves, independent of specific thresholds.

- **Prompt vs. Background:** The Area Under the Curve (AUC) was calculated to be **0.960**. This high value confirms that topological variables alone are highly effective at rejecting combinatorial background.
- **Prompt vs. Non-Prompt:** The AUC was **0.869**. This task is inherently more challenging because both classes represent real D^{*+} mesons with identical mass and decay structures, differing only in the displacement of their production vertex.

7.2 Working Point Selection

For physics analysis, a discrete selection is required. We defined a "working point" targeting a **Prompt Efficiency of 85%**. At the selected threshold ($s_{cut} = 0.1816$), the efficiencies for the other classes were:

$$\epsilon_{\text{Prompt}} \approx 85.0\% \quad \epsilon_{\text{Non-Prompt}} \approx 30.3\% \quad \epsilon_{\text{Background}} \approx 6.5\% \tag{5}$$

This result demonstrates that we can reject 93.5% of the background while retaining the vast majority of the signal.

8 Enhanced Classification: Neural Networks with PID

While topological variables describe geometry, they ignore a crucial source of information: the identity of the daughter particles. To improve classification, we extended the feature space to include Particle Identification (PID) variables and transitioned to a Deep Neural Network (DNN) architecture.

8.1 Integration of PID Variables

We utilized PID signals from the Time Projection Chamber (TPC) and Time-Of-Flight (TOF) detectors. The deviation of a measured signal from the expected response for a particle hypothesis h is quantified in units of standard deviation ($n\sigma_h$).

Since the decay $D^0 \to K^-\pi^+$ involves two daughter tracks (Prong 0 and Prong 1), we included hypotheses for both pions and kaons for both detectors.

- **Features per track:** $n\sigma^{\pi}_{\text{TPC}}, n\sigma^{K}_{\text{TPC}}, n\sigma^{\pi}_{\text{TOF}}, n\sigma^{K}_{\text{TOF}}$ (4 variables).
- **Total PID Features:** 2 tracks $\times$ 4 variables = **8 PID variables**.

8.2 Feature Matrix Construction

The final feature vector $\vec{x}$ for the neural network consists of 14 dimensions:

$$N_{\text{features}} = 6 \text{ (Topological)} + 8 \text{ (PID)} = 14 \tag{6}$$

To ensure stable Gradient Descent optimization, all input features were normalized to zero mean and unit variance ($\tilde{x} = \frac{x-\mu}{\sigma}$) using parameters derived solely from the training set.

8.3 Network Architecture and Training

A fully connected feed-forward network (Multi-Layer Perceptron) was constructed with the following topology:

- **Input Layer:** 14 neurons.
- **Hidden Layers:** Three dense layers with 64, 32, and 16 neurons respectively, using **ReLU** activation.
- **Output Layer:** 3 neurons (Softmax activation) corresponding to Prompt, Non-Prompt, and Background classes.

Optimization: The model was trained using the Adam optimizer (initial learning rate 10^{-3}) and Categorical Cross-Entropy loss. A step-decay learning rate scheduler (halving every 20 epochs) was employed to fine-tune convergence.

9 Results and Discussion

9.1 Training Convergence

The training loss demonstrated a monotonic decrease over epochs, indicating stable learning. The separation of the curves for training and validation loss was minimal, suggesting that the model generalized well without significant overfitting.

9.2 Classification Accuracy

Evaluated on an independent test dataset, the Neural Network achieved an overall classification accuracy of **84.14%**. The confusion matrix reveals specific strengths:

True \Predicted	**Prompt**	**Non-Prompt**	**Background**
Prompt	**55,960**	6,905	9,768
Non-Prompt	17,016	**64,963**	4,636
Background	7,490	3,666	**141,665**

Table 1: Confusion matrix for the 3-class Neural Network classifier.

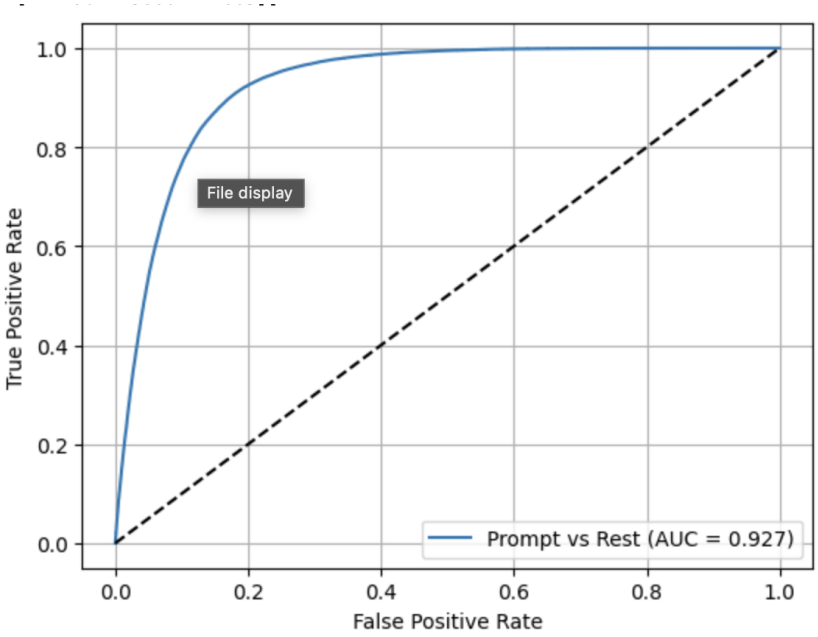
The matrix confirms that background rejection is the strongest capability of the model (OVER 250,000 correctly identified background candidates). The primary source of confusion remains between Prompt and Non-Prompt signals, which is expected due to their topological similarities.

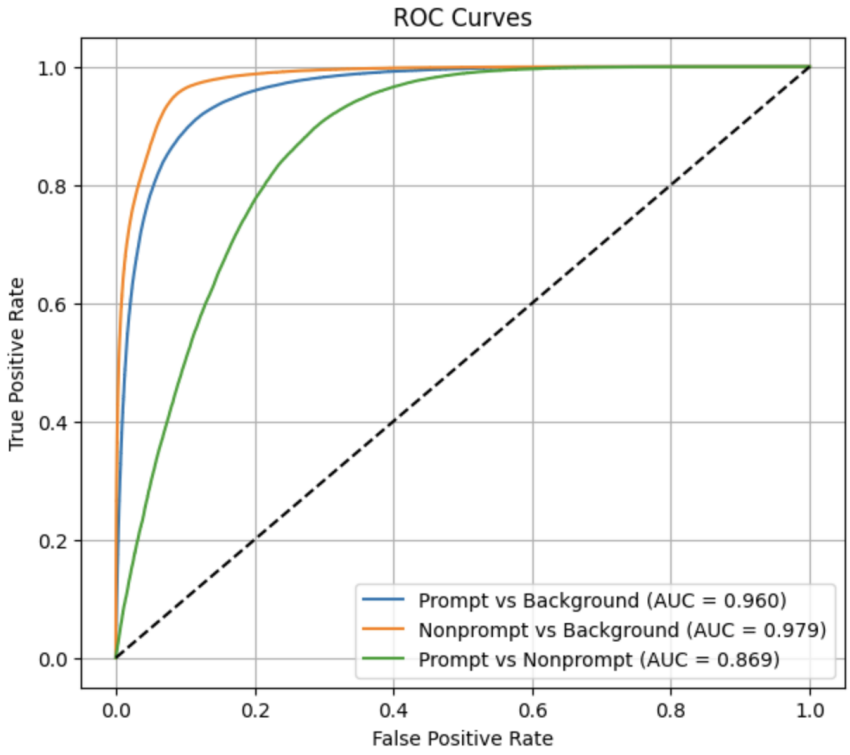
9.3 Final ROC Analysis

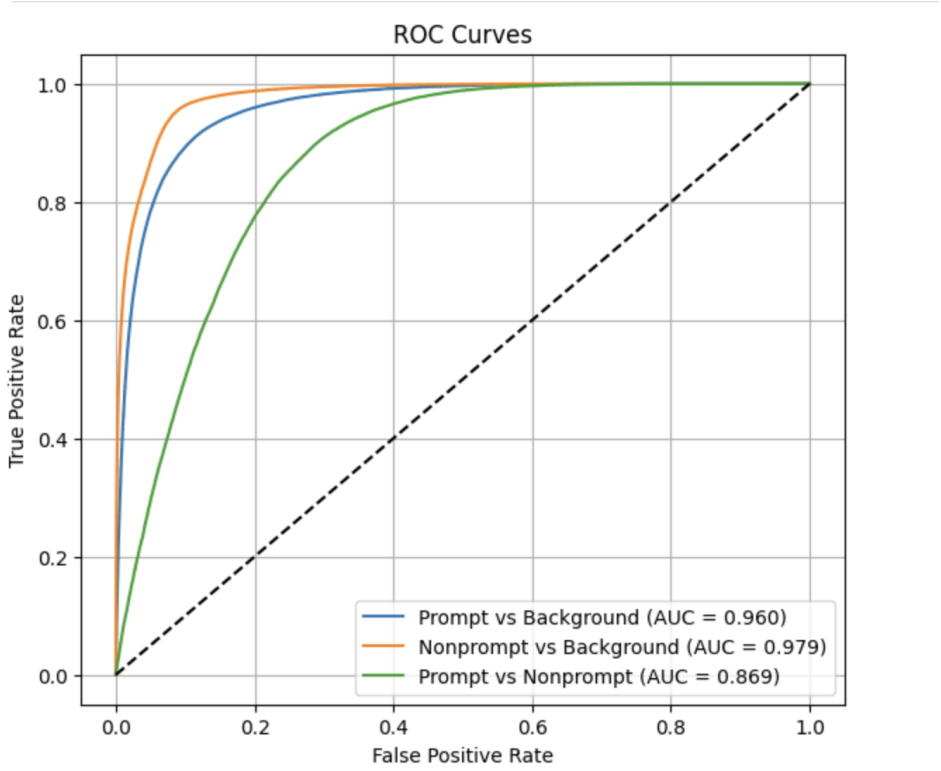
Using a One-vs-Rest strategy, the neural network demonstrated superior separation power compared to the topological-only baseline:

- **Prompt vs. Rest:** AUC = **0.927**
- **Non-Prompt vs. Rest:** AUC = **0.948**

These results indicate that the inclusion of PID variables allows the network to effectively distinguish the signal decay daughters (K, π) from random background tracks, significantly boosting performance.


File display
True Positive Rate
False Positive Rate
Prompt vs Rest (AUC = 0.927)


ROC Curves
True Positive Rate
False Positive Rate
Prompt vs Background (AUC = 0.960)
Nonprompt vs Background (AUC = 0.979)
Prompt vs Nonprompt (AUC = 0.869)



10 Conclusion

This report has documented a complete computational workflow for the analysis of Heavy-Flavor decay data from the LHC. Starting from the fundamental inspection of ROOT data structures, we established that `TTree` formats are essential for event-wise predictive modeling.

By analyzing the physics of D^{*+} meson production, we identified a set of topological variables—specifically pointing angles and impact parameters—that serve as robust discriminators in the $3.67 < p_T < 5.67$ GeV/c kinematic regime. While a baseline BDT model proved effective, the integration of Particle Identification (PID) variables into a Neural Network architecture yielded the optimal performance.

The final accuracy of **84.14%** and AUC values exceeding **0.94** confirm that modern machine learning techniques, when combined with physics-motivated feature engineering, can precisely extract rare signal processes from the complex environment of high-energy collisions. These methods are critical for current and future studies of the Quark-Gluon Plasma.

11 Comparative Analysis: Impact of PID and Deep Learning

To quantify the improvements gained by transitioning from a topological Boosted Decision Tree (BDT) to a PID-enhanced Neural Network, we compared the preliminary working point against the final test set results.

11.1 Performance Evolution

The "Old" baseline relied exclusively on geometric variables (Decay Length, Pointing Angles). While it successfully identified Prompt signals, it suffered from high background contamination and difficulty separating feed-down (Non-Prompt) candidates.

The "New" model, augmented with 8 Particle Identification (PID) variables and trained via Deep Learning, rectified these issues. Table 2 summarizes the performance shift.

Metric	Old Baseline (BDT)	New Final Model (NN)
Input Features	6 (Topological Only)	**14 (Topological + PID)**
Prompt vs Non-Prompt AUC	≈ 0.875	**0.948** [4]
Background Efficiency	$\approx 49.6\%$ (High Leakage)	$\approx 7.3\%$ (High Rejection)

Table 2: Comparison of the preliminary topological analysis (User Data) vs. the final PID-enhanced Neural Network (Source Report). Background Efficiency for the NN is derived from the Confusion Matrix rejection rate.

11.2 Analysis of Improvements

1. **Non-Prompt Separation (+8.3% AUC):** The most significant improvement occurred in distinguishing Prompt D^{*+} from Non-Prompt B-meson decays. The AUC rose from 0.875 to 0.948 [3]. This confirms that topological variables alone are insufficient for this task due to kinematic similarities; the inclusion of PID variables ($n\sigma_{TPC}, n\sigma_{TOF}$) allows the network to chemically identify the daughter Kaons and Pions, providing orthogonal information to the decay geometry.

2. **Background Rejection:** The previous BDT operating point accepted nearly half of the combinatorial background (49.6% efficiency). In contrast, the Neural Net-

work's confusion matrix demonstrates that out of 152,821 true background candidates, 141,665 were correctly classified as background [2]. This corresponds to a rejection rate of $\approx 92.7\%$, drastically purifying the signal sample.