AFB studies at 500 GeV

LCFI+ Flavour Tag Optimization

ILD Software & Analysis meeting
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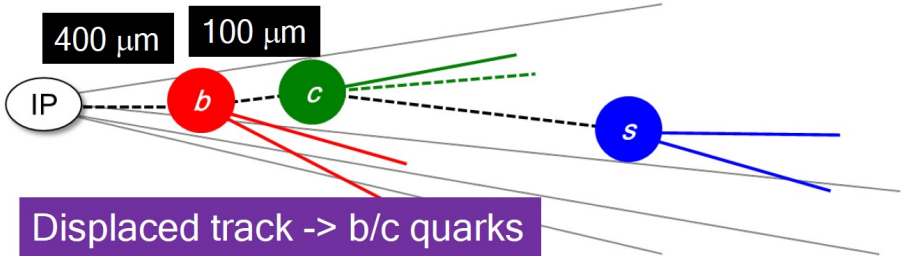
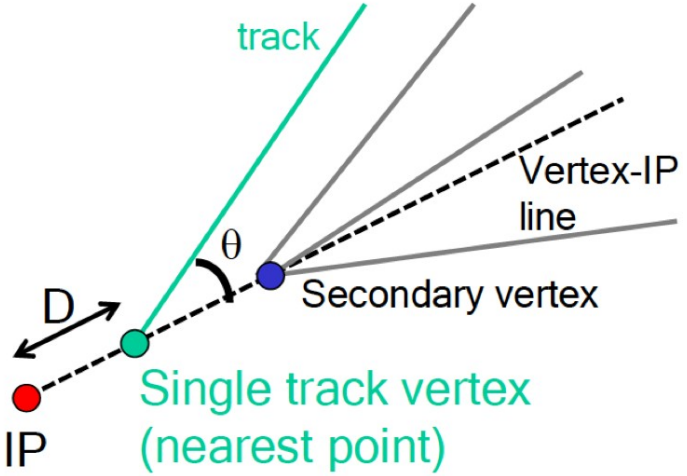
LCFI+ (vertexing)

LCFI+ (Taikan Suehara, Tomohiko Tanabe; arXiv:1506.08371) :

- Vertex finder:
  - Reconstruct collinear or close-to-collinear vertexes by merging particle tracks from the event information.
  - Distance ($\tau_q \cdot c$) from the IP is key for b and c quark ID: Displaced vertexes.
  - We also encounter single track vertexes: pseudo-vertexes.
  - There are more details to select the tracks used for quark id.
    - e.g. V^0 rejection for neutral particles.

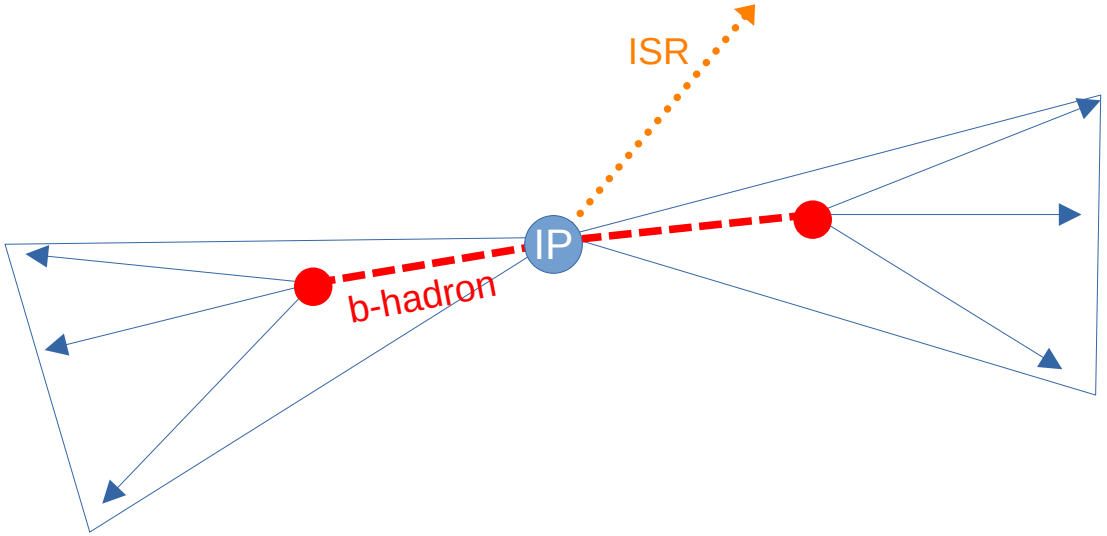




LCFI+ (jet clustering)

LCFI+ (Taikan Suehara, Tomohiko Tanabe; arXiv:1506.08371) :

- Jet Clustering:
  - Use the vertexing information.
  - Different algorithms could be used (k_T, Durham, **VLC**, etc.).
  - In our case, we expect two back-to-back jets with ISR:



TMVA in LCFI+

- Most of the variables used in the TMVA are derived from d0, z0, the number of vertexes, the number of pseudo-vertexes and other kinematical variables (like r-phi plane or p_T).
  - e.g. b-quark probability in d0 values for all tracks.
- Classification in categories:
  - The training is performed 4 times (A, B, C, D), *in a single run* , with different selection of vertexing and single track pseudo-vertexing.

Category	A	B	C	D
Number of vertices	0	1	1	2
Number of single-track pseudovertices	0-2	0	1	0

Particle Swarm Optimization (PSO)

- Iterative method to optimise a machine learning classification.
  - In our case, to optimise the multi-class BDT (Boosted Decision Tree) used for flavour tagging in LCFI+ (see back-up for more).

- The final goal is to obtain new weights for b-tagging and c-tagging.
  - Ideally, these would have the best performance, while avoiding overtraining.

- We checked $q\bar{q}$ simulated events at different energies:
  - 250 GeV: Small samples for a first testing.
  - 500 GeV: Big samples (new simulations), main working horse.

1 optimization per LCFI+ category

Boosted Decision Trees (BDT) - TMVA

- We are already working with these Gradient Boosted Decision trees using ROOT's Toolkit for MultiVariate data Analysis (TMVA). We use the following parameters:
  - BoostType=Grad.
  - NTrees.
  - Shrinkage.
  - UseBaggedBoost:BaggedSampleFraction.
    - Bagging: A new sampling is performed before each step (removes biases).
  - NCuts (binning used when sampling).
  - MaxDepth (Nº of leaves).

The Particle Swarm Algorithm optimizes the use of *these parameters*

We used all but the orange ones, which are method definitions

PSO - Overview

- Particle Swarm Optimization is a Gradient-free, bio-inspired, stochastic, population-based algorithm to optimize any kind of process towards a certain goal:
  - No maths involved in the optimization (no gradients or loss functions!).
  - It just try configurations and saves the *best-performing one*.
    - It mimics how animals look for resources, by trial and error.

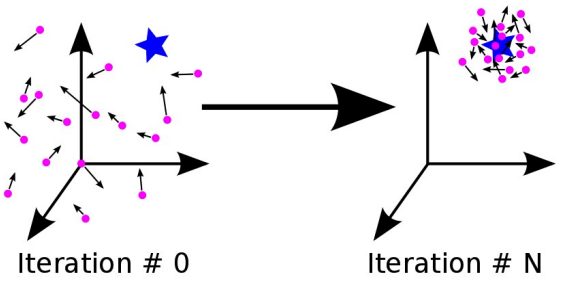


Image taken from a website

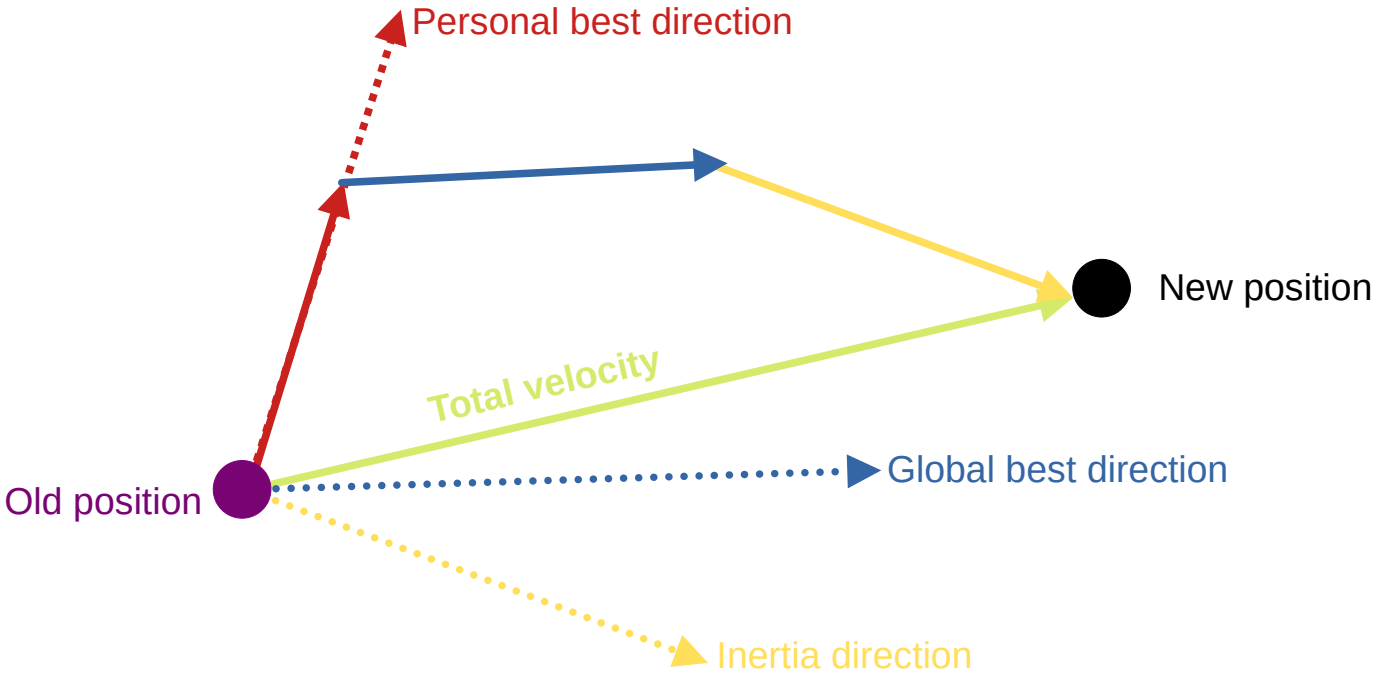
- How it works:
  - We have N “particles” (in our case: configurations of the BDT). Then:
    1) The BDT runs with the configuration of the particle.
    2) When finished, each particle gets a performance score.
       -We define a Function Of Merit (FOM) for this scoring
    3) We track each particle’s best configuration and the best global one.
    4) The particles move to a new configuration (next slide).

For each iteration

PSO - Overview

Position: $\overrightarrow{X_i^{t+1}} = \overrightarrow{X_i^t} + \overrightarrow{V_i^{t+1}}$

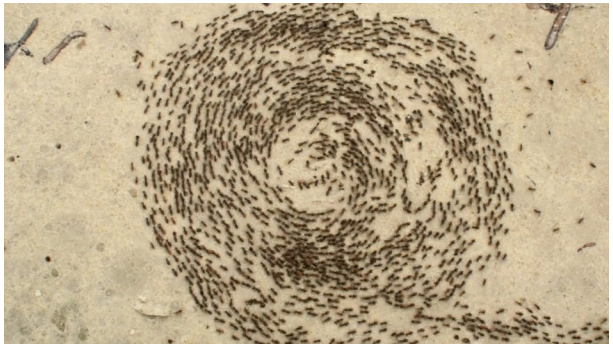
Velocity: $\overrightarrow{V_i^{t+1}} = w\overrightarrow{V_i^t} + c_1 r_1 \left(\overrightarrow{P_i^t} - \overrightarrow{X_i^t}\right) + c_2 r_2 \left(\overrightarrow{G^t} - \overrightarrow{X_i^t}\right)$



PSO – Adaptation to FT in LCFI+

- We need:
  - A 3-class classifier (b quarks, c quarks, uds quarks).
  - We also want to avoid overfitting:
    - Kolmogorov-Smirnov test
    - Anderson-Darling test

    Control biased test scores. (more info in back-up)
  - We need a FOM adapted to 3 different classes.
  - Important remark: A final check is **always needed**:



Trial and error can go wrong sometimes!

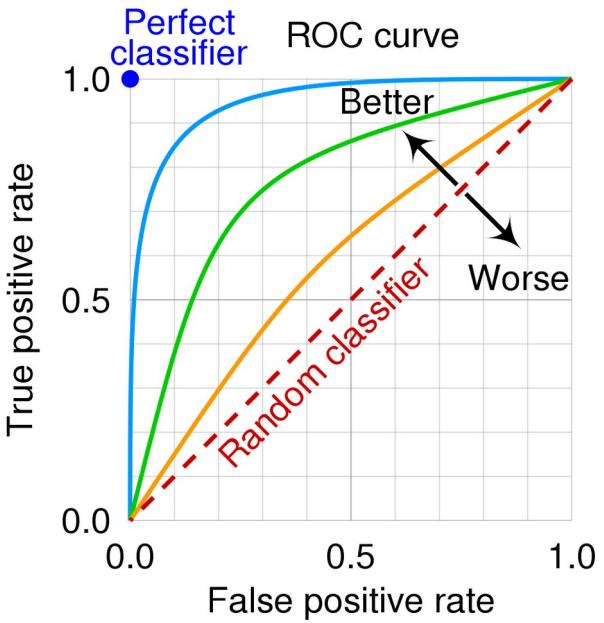
PSO – Function Of Merit (FOM)

- The FOM being used is the averaged value of the Integral of the Receiver Operating Characteristic curve for each of the 3 data classes.
  - Considering the target class as signal and the others as background.

- Our FOM is simply:

$$FOM = (AUC[b_{quark}] + AUC[c_{quark}] + AUC[uds_{quarks}]) / 3,$$

where AUC = ”Area Under Curve” (ROC Integral).



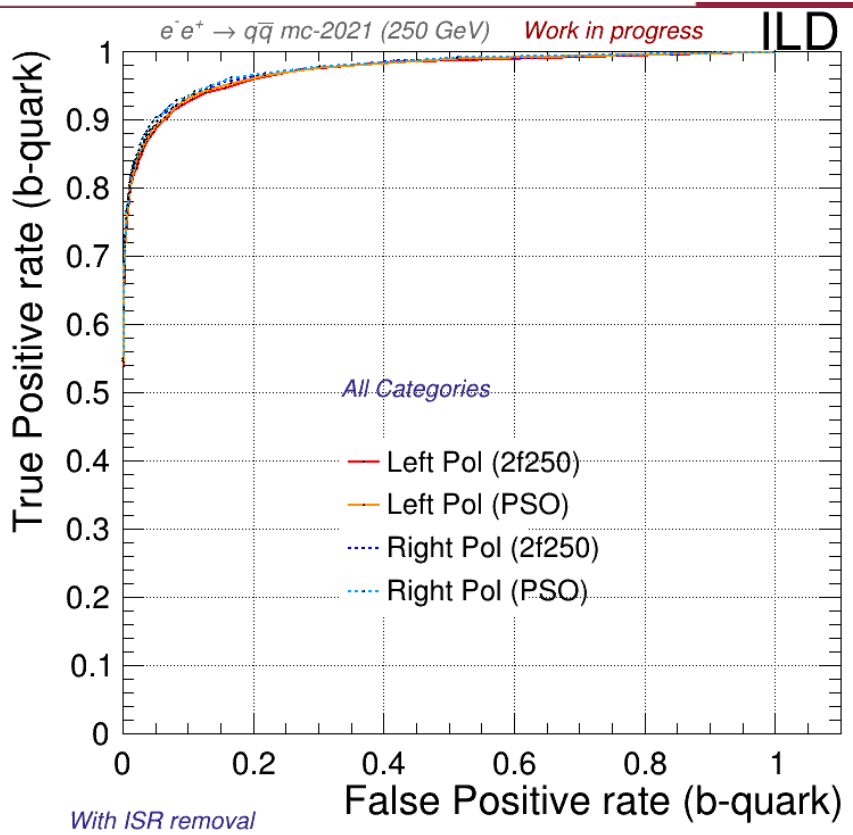
PSO – Performance plots

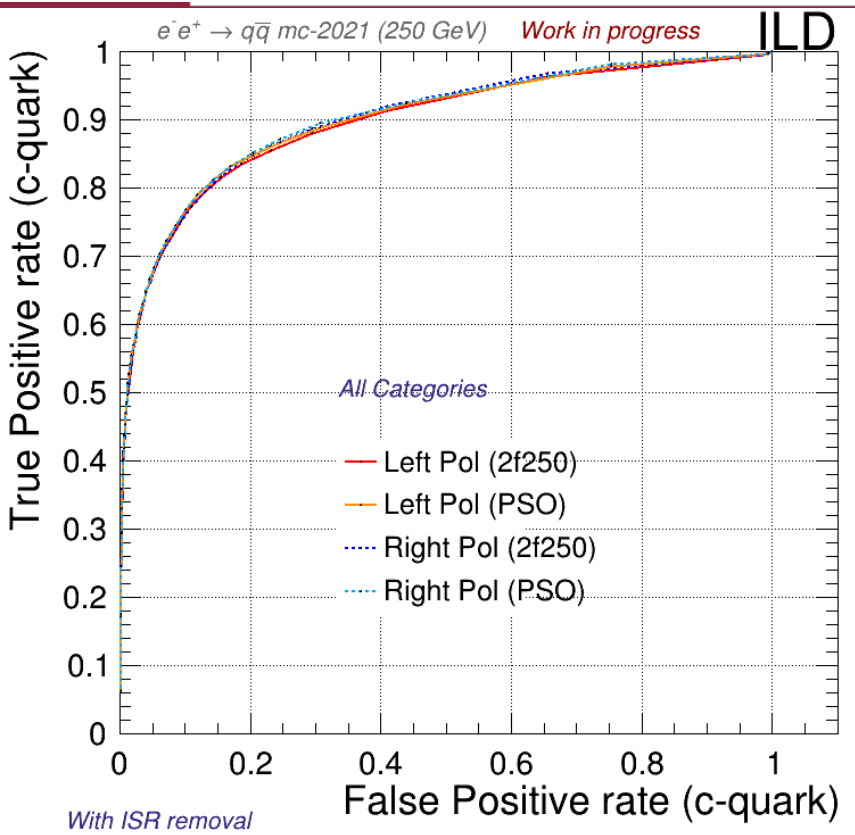
- On the next slides:
  - Plots for b-tag and c-tag:
    - ROC, considering the desired flavour as signal and the others as background.
      - Also approximated AUC (ROC Integral) values to compare
    - Purity vs Efficiency.
  - Luminosities:

PSO
PSO (pol. test)

$e^-_L e^+_R$	20 fb^{-1} (2.5 M events)	1.6 fb^{-1} (200 K events)
250 GeV	Test + Training (50/50)	Sample for plots
$e^+_R e^+_L$	36 fb^{-1} (2.5M events)	2.8 fb^{-1} (200 K events)
$e^-_L e^+_R$	250 fb^{-1} (1.2M events)	1430 fb^{-1} (7.0 M events)
500 GeV	Test + Training (50/50)	Independent sample for plots
$e^+_R e^+_L$	480 fb^{-1} (1.5M events)	1060 fb^{-1} (3.2 M events)

PSO Performance (250 GeV)

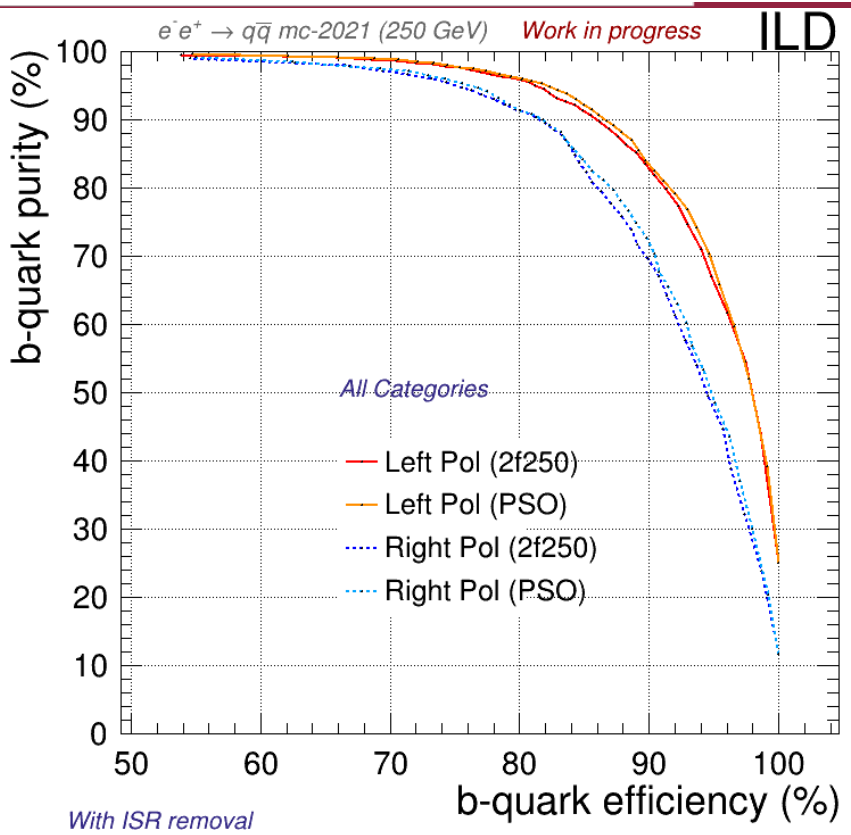


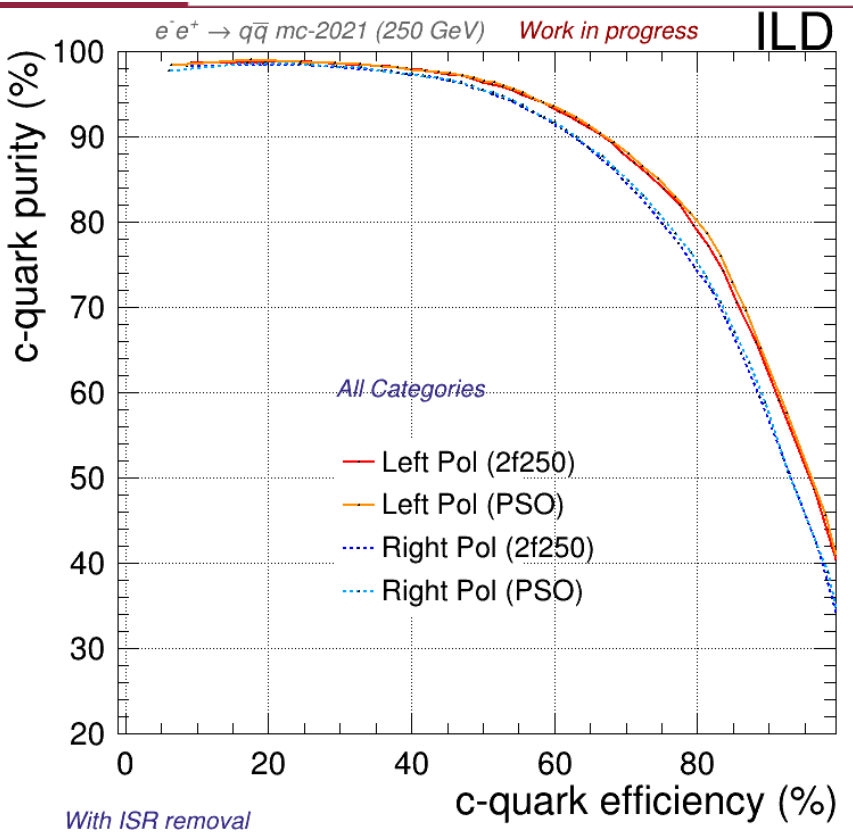


[Integrals 2f250] e^-_L: 0.971 | e^-_R: 0.973
[Integrals PSO] e^-_L: 0.973 | e^-_R: 0.976

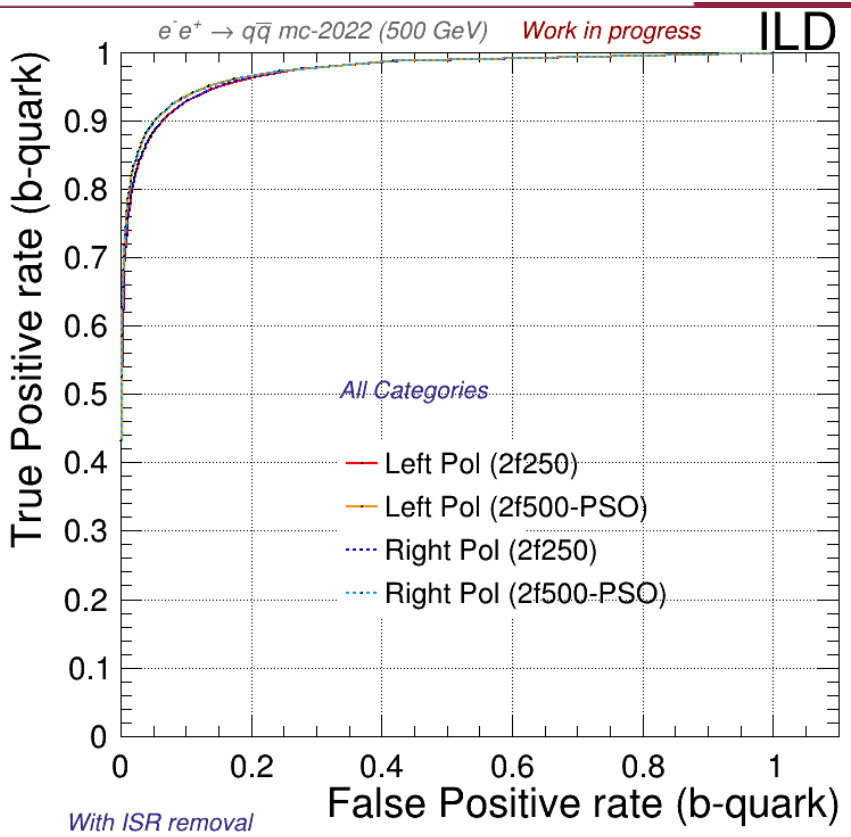
[Integrals 2f250] e^-_L: 0.898 | e^-_R: 0.902
[Integrals PSO] e^-_L: 0.901 | e^-_R: 0.904

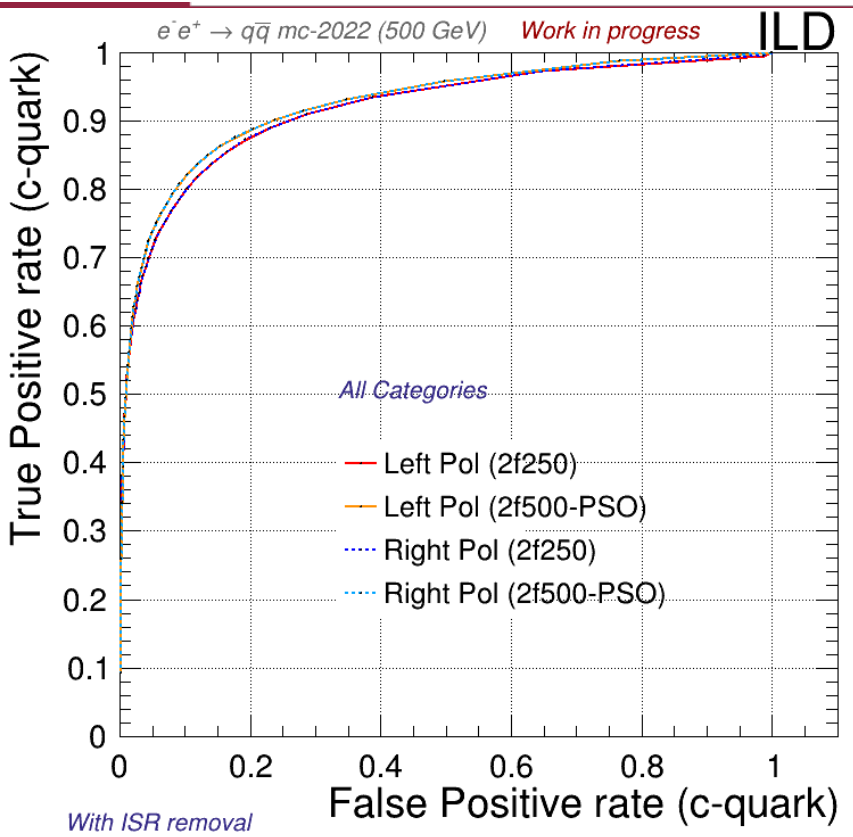
PSO Performance (250 GeV)





PSO Performance (500 GeV)

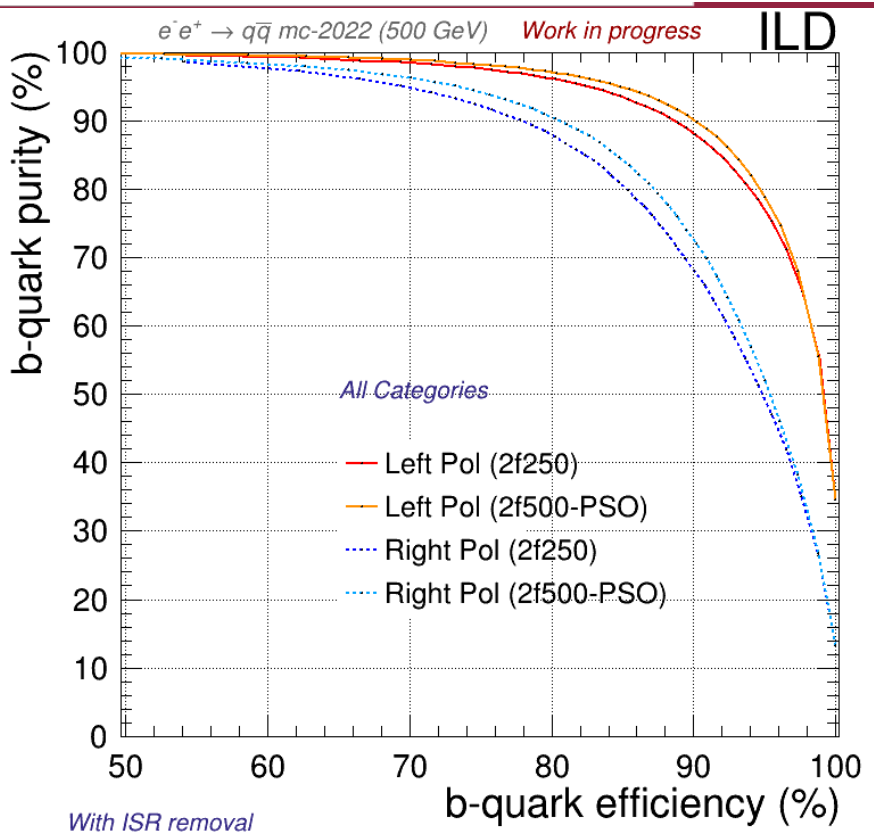


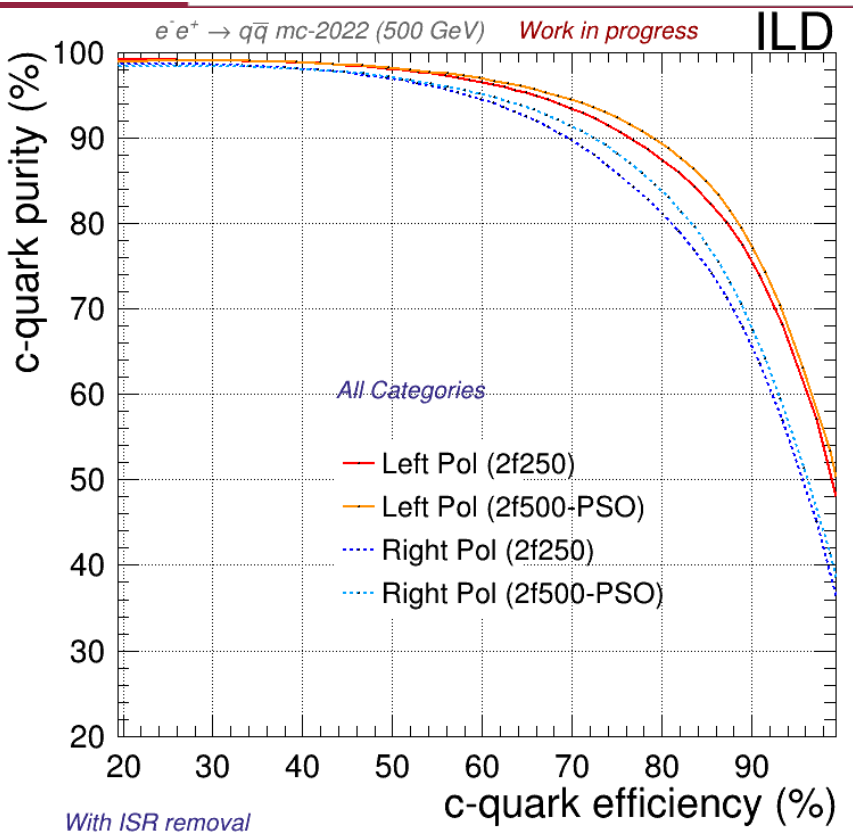


[Integrals 2f250] e^-_L: 0.972 | e^-_R: 0.971
[Integrals PSO] e^-_L: 0.974 | e^-_R: 0.974

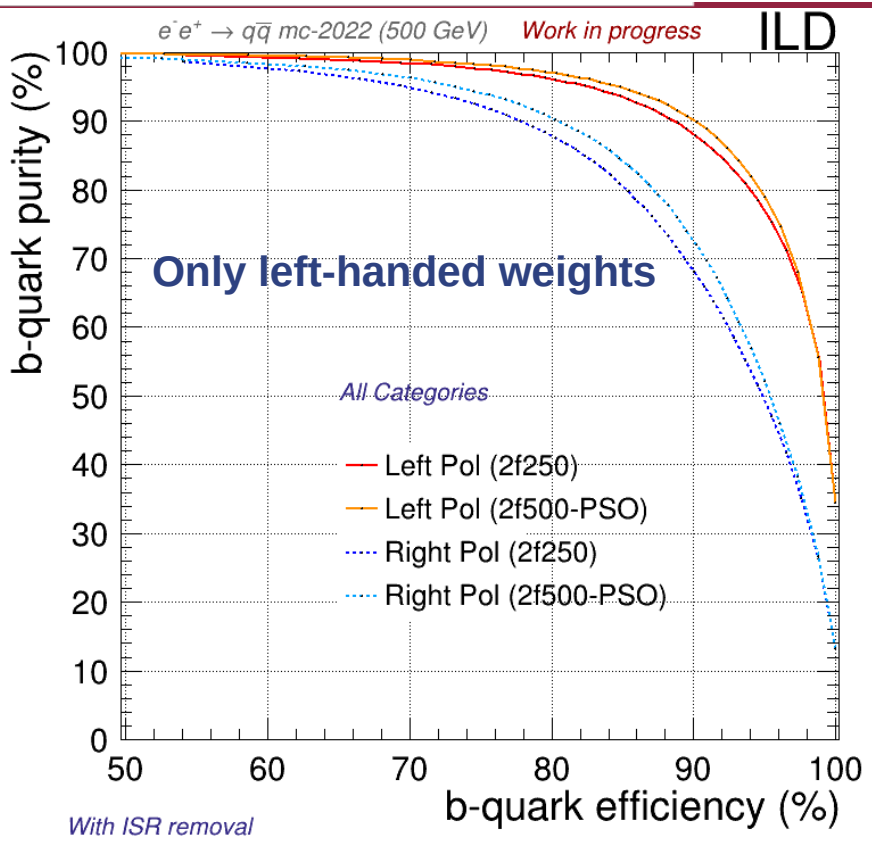
[Integrals 2f250] e^-_L: 0.917 | e^-_R: 0.917
[Integrals PSO] e^-_L: 0.925 | e^-_R: 0.925

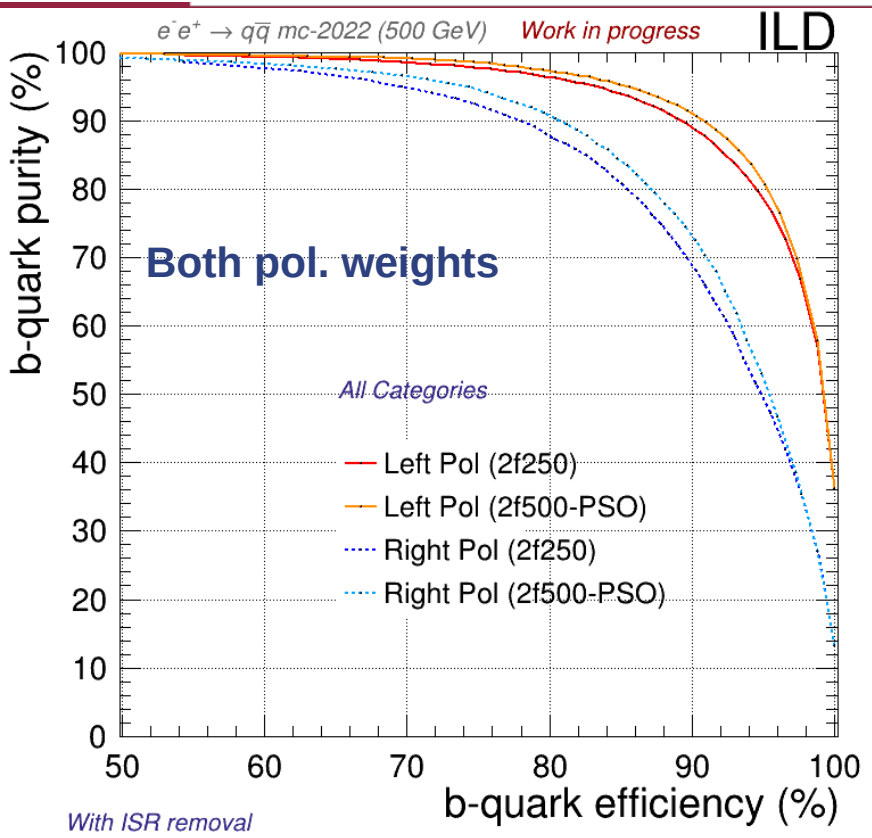
PSO Performance (500 GeV)





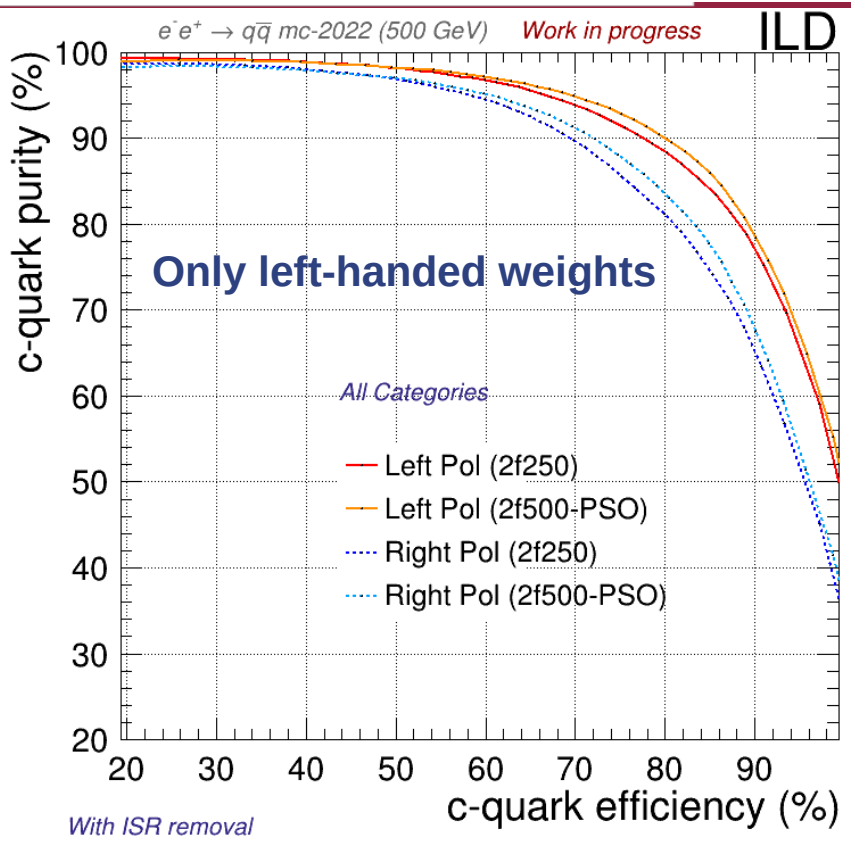
Polarization dependence (500 GeV)

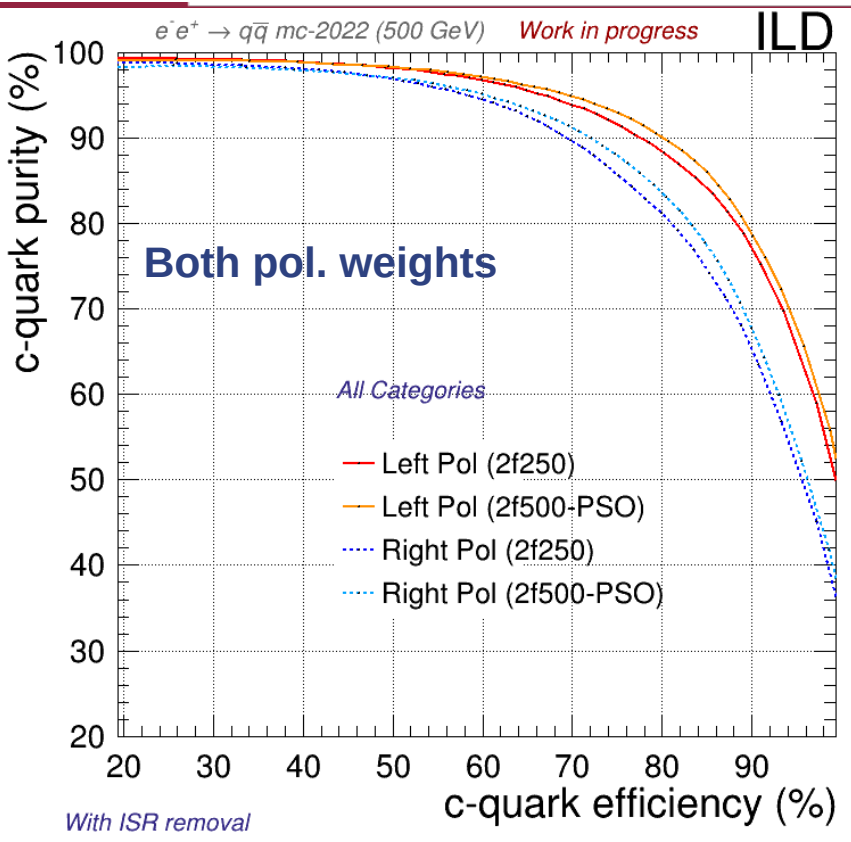




Minimal impact when training with sets of specific polarization

Polarization dependence (500 GeV)





Minimal impact when training with sets of specific polarization

PSO Performance - Conclusions

- We can notice:
  - An improvement in b-tag and c-tag for all categories and in the global performance.
  - The impact in efficiency if we train for different polarizations is very small.
    - The impact of the general PSO optimization is way greater.

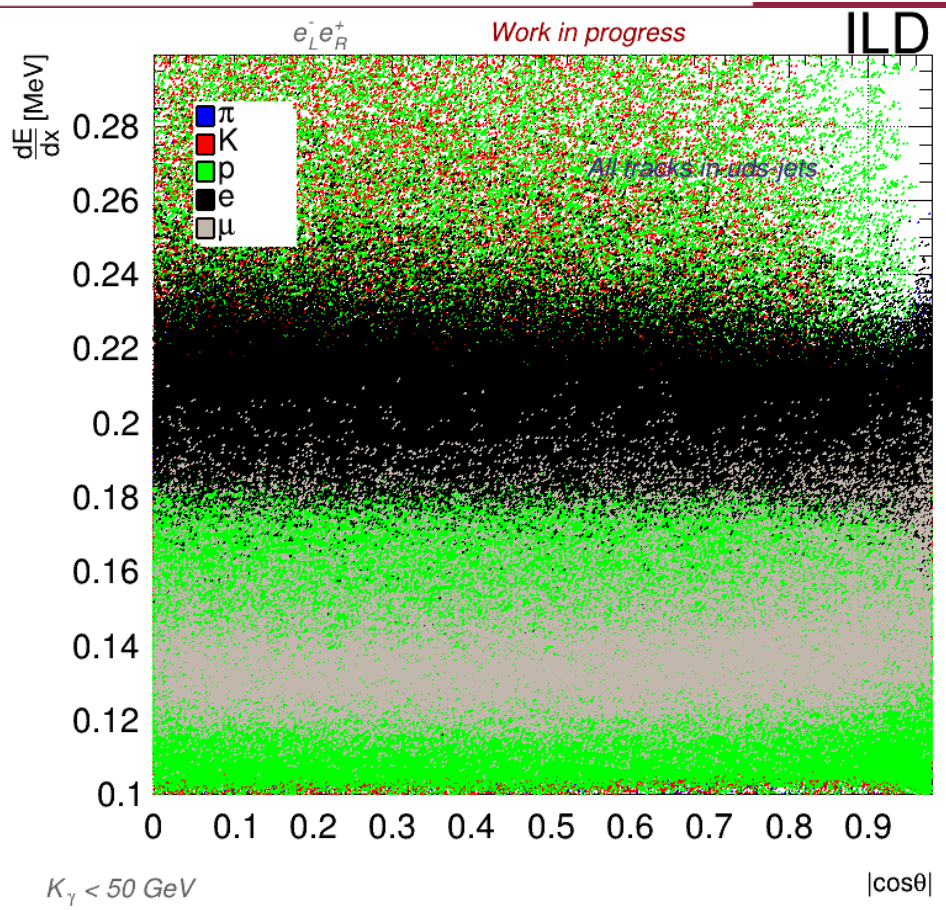
- Now we are going beyond this optimization by introducing new variables in LCFI+.
  - Observables derived from dEdx (next slides).
    - Work in progress!

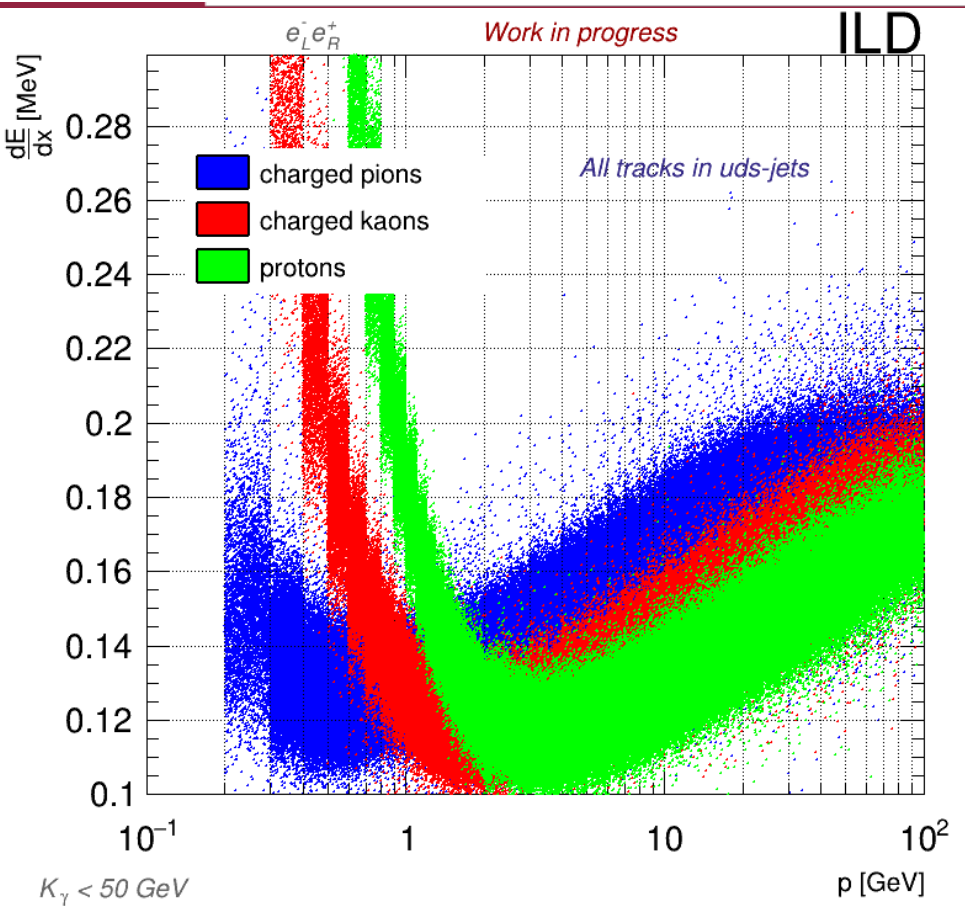
Using dEdx for flavour tagging

- We will study the *distance* of different tracks wrt Kaon dE/dx:
  - 1 pfo in a single track → 1 particle energy trace (Bethe-Bloch formula).
  - Our .lcio files already have an estimation of the distance between a given track and the estimated for a given particle (Kaon, pion, etc.).
    - This distance is not always a good estimation: we have to preselect first a region in momenta in which this measurement is consistent.

- Once the distance is proved to be somehow useful to distinguish different particles:
  - Building new observables useful for flavour tagging!

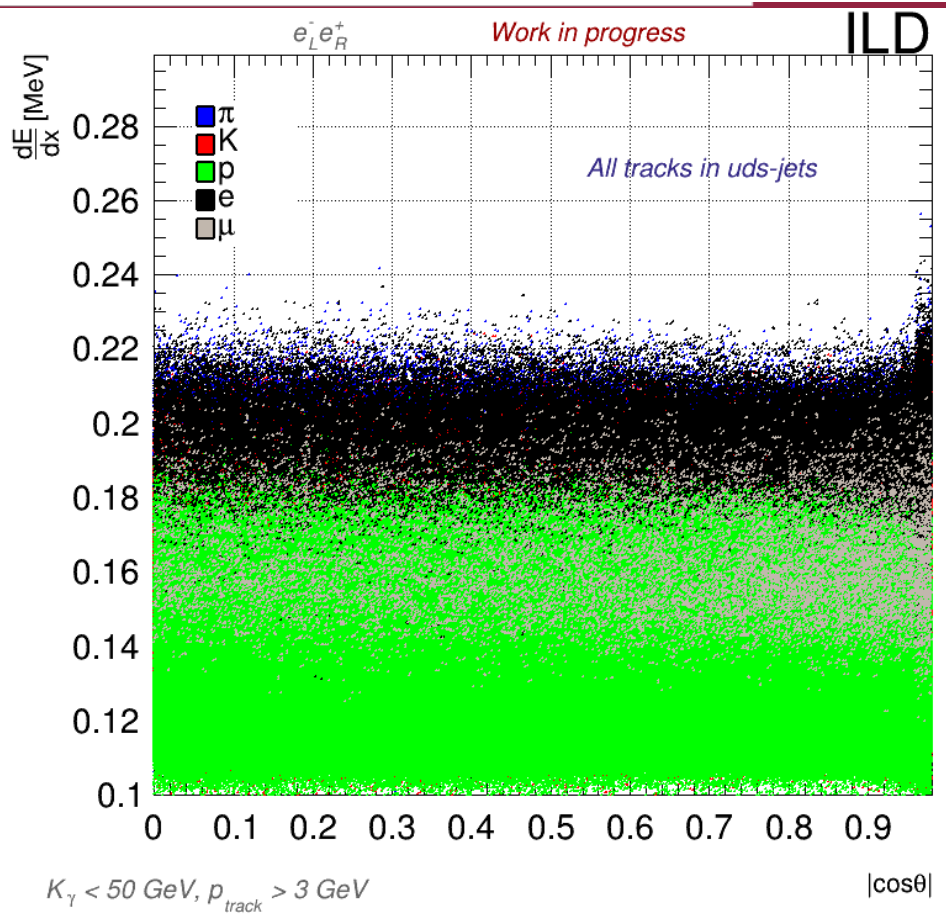
dEdx – Momentum distribution

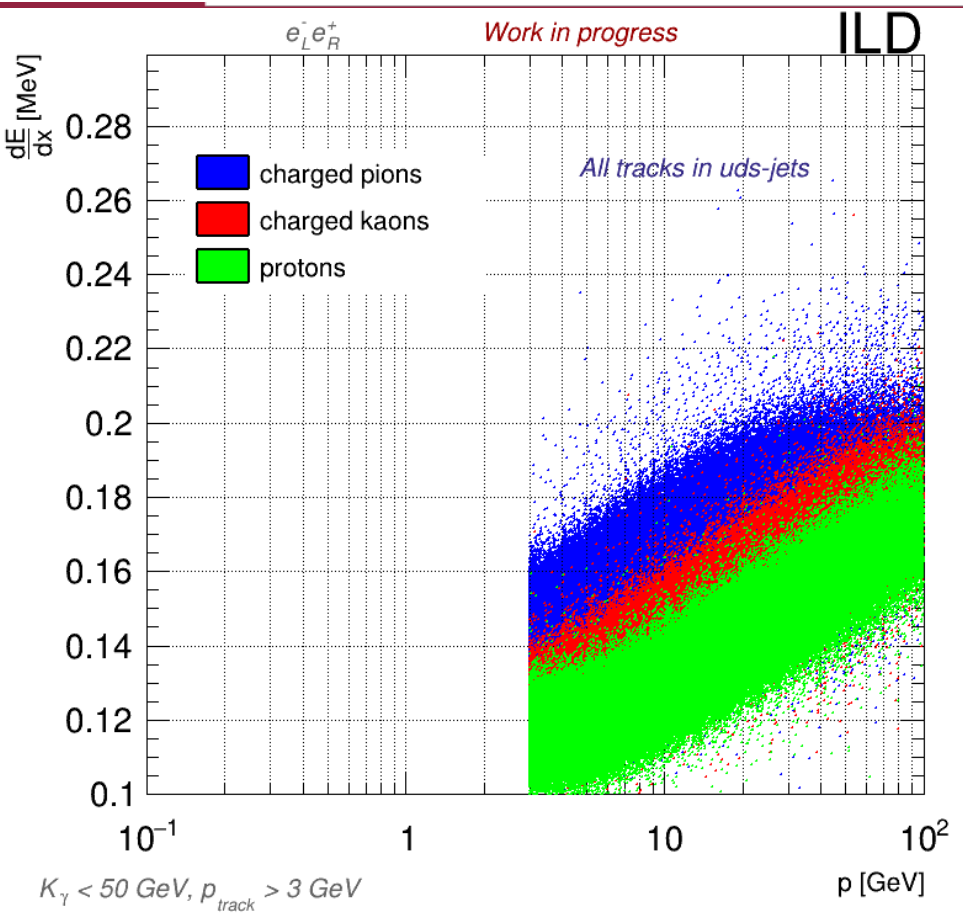




There's a high population at low momentum and below 3 GeV the distributions overlap!

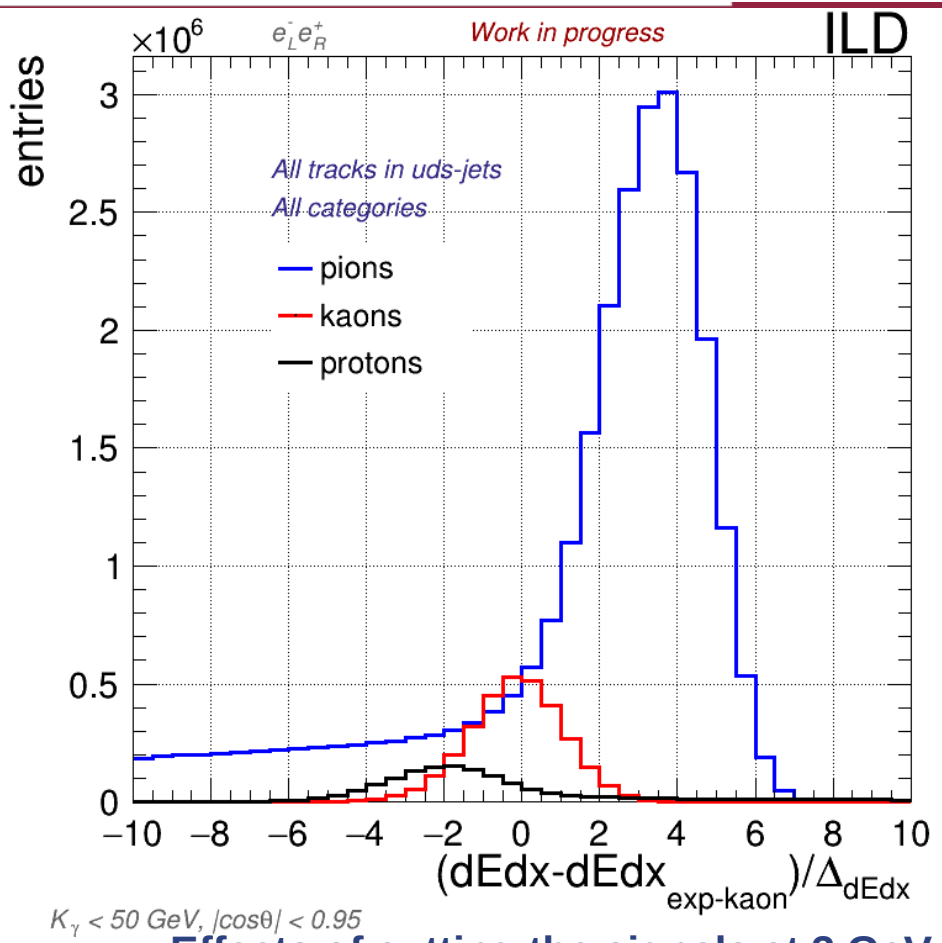
dEdx – Cut in tracks' momentum

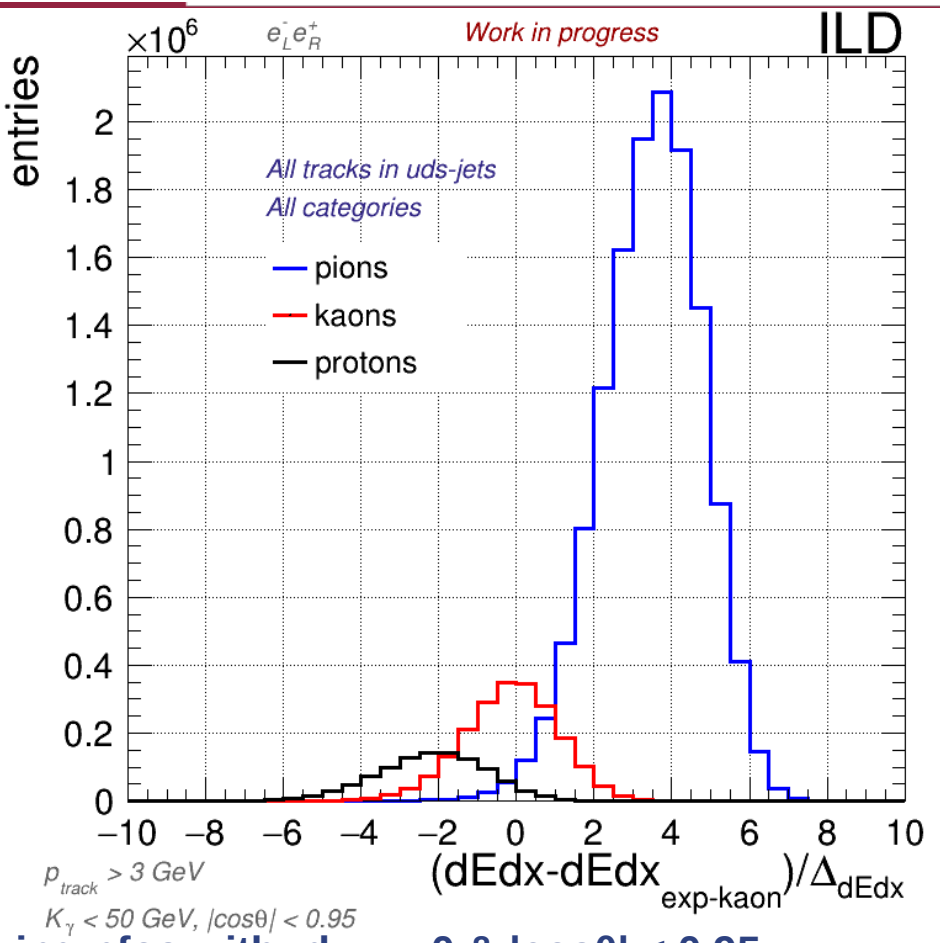




Effects of cutting the signals at 3 GeV. This behavior is similar to b and c jets.

dEdx – Kaon Distance Significance (KDS)

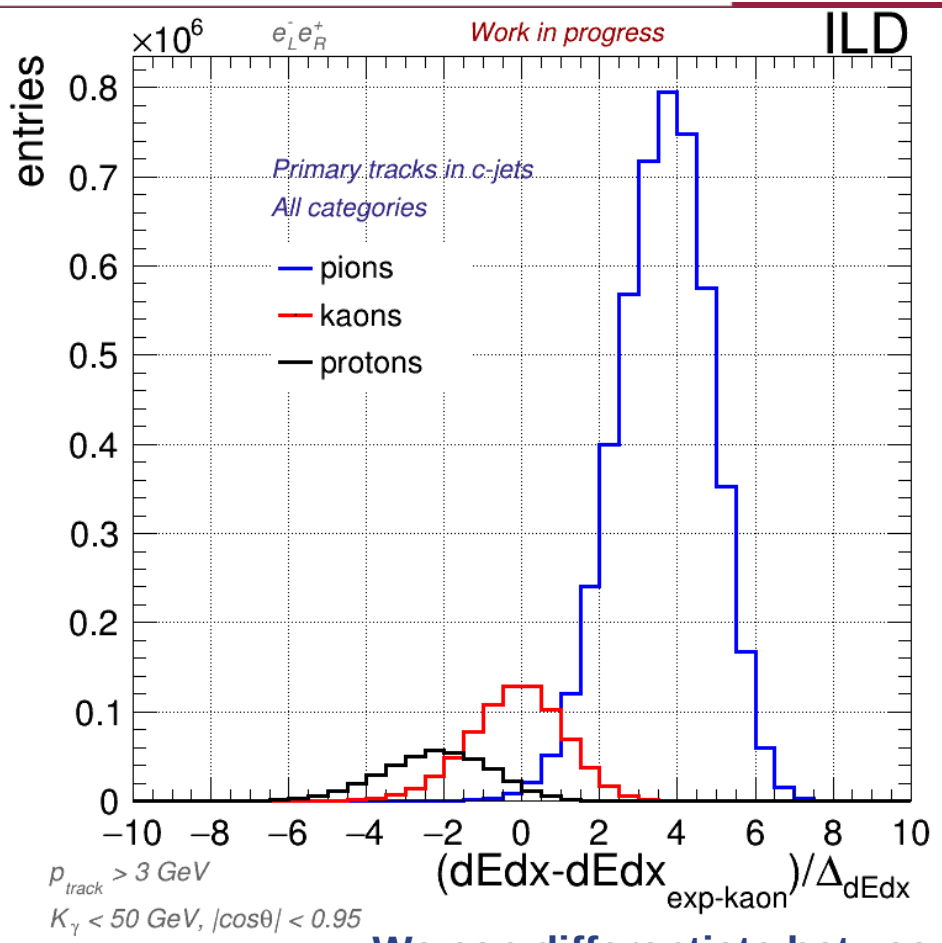


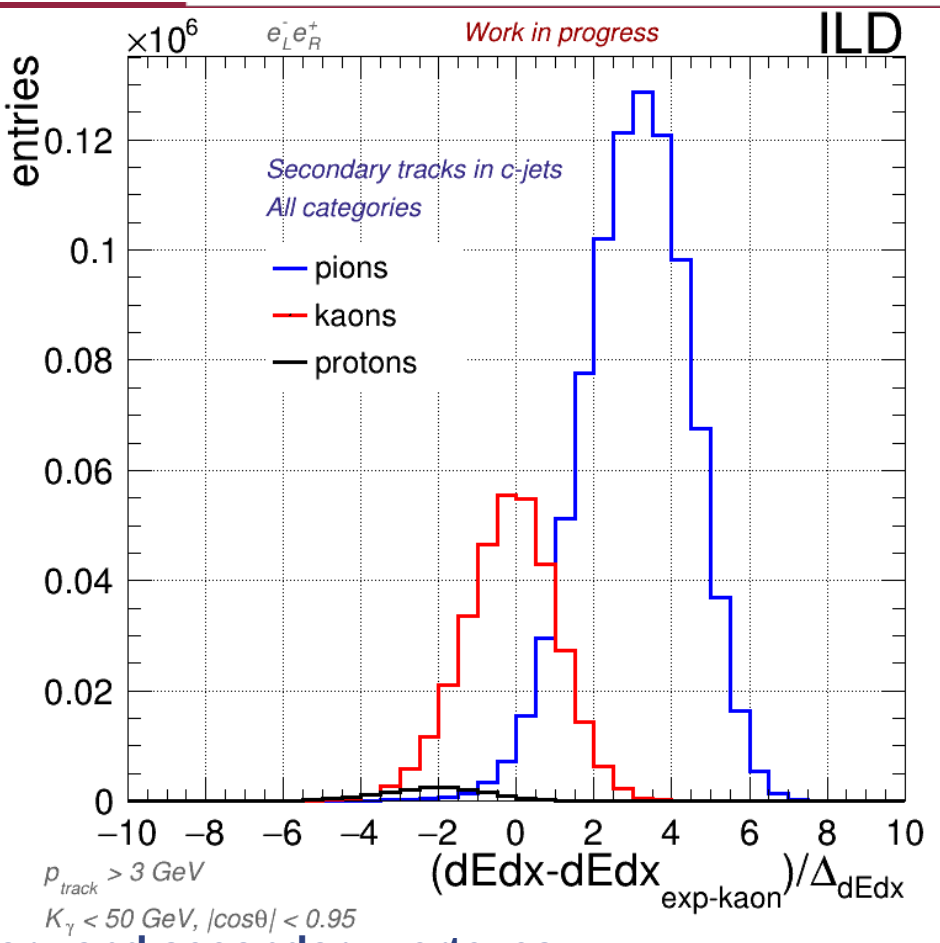


Effects of cutting the signals at 3 GeV, removing pfos with [1]d_{kaon} = 0 & |cosθ| < 0.95

1. A peak appeared at d=0. Probably an initialization issue in *dEdxKaonDistance*. *Plots in back-up slides.*

dEdx – KDS in primary and secondary vtx.





We can differentiate between primary and secondary vertexes

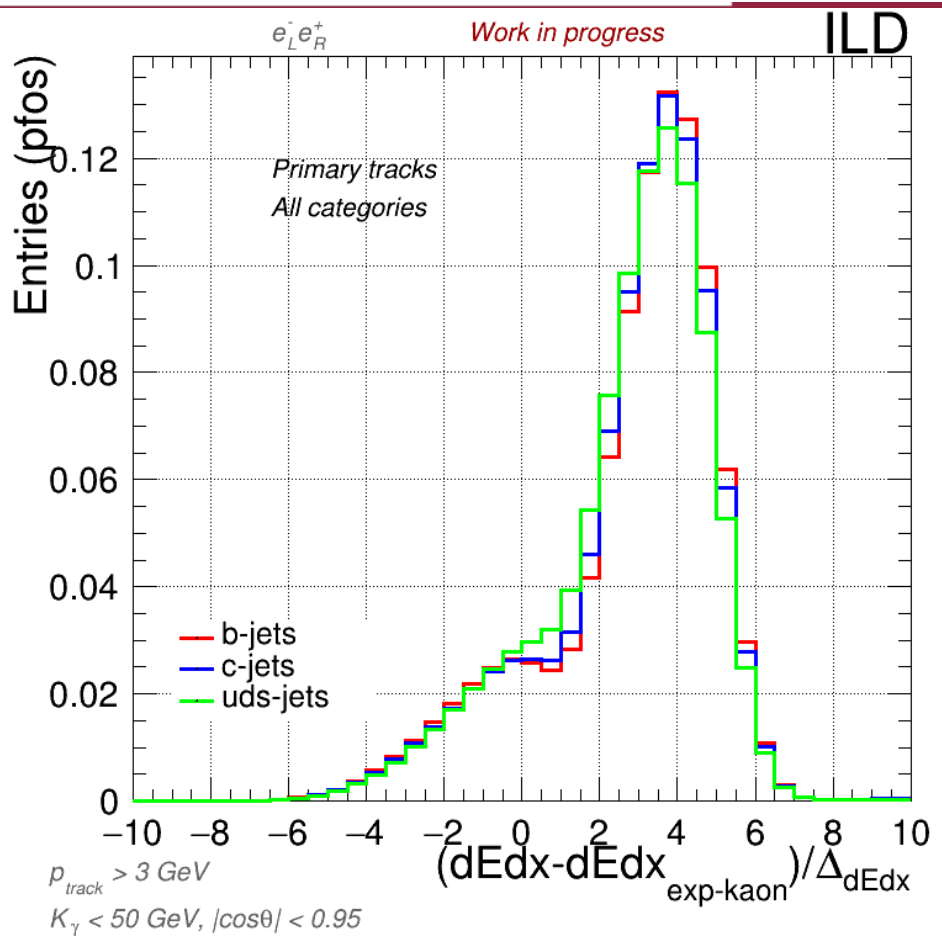
dEdx – Moving to real observables

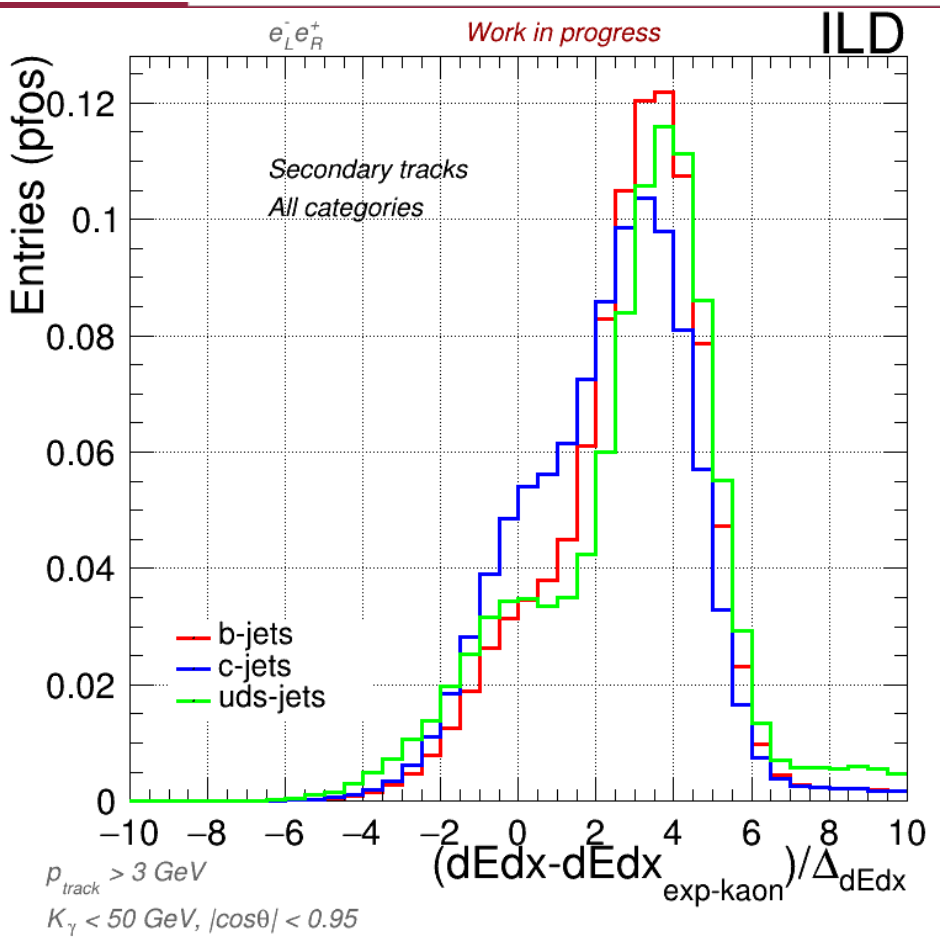
- Now that we have some hints about differences in pfos' dEdx distributions we need:
  - Distributions that allow an inference about the content of *1 single jet*.

- On the next slides we will see:
  - Histograms of untagged pfos' dEdx distance to kaon's dEdx experimental expected value.
    - Also, histograms for one *a priori* classification of pfos according to such distance: negative, null or positive distance.
      - I called these particles "Estimated protons, kaons or pions".
  - Observables using ratios between these estimated particles:
    - Estimated K/p.
    - Estimated π/p.
    - Estimated π/K.

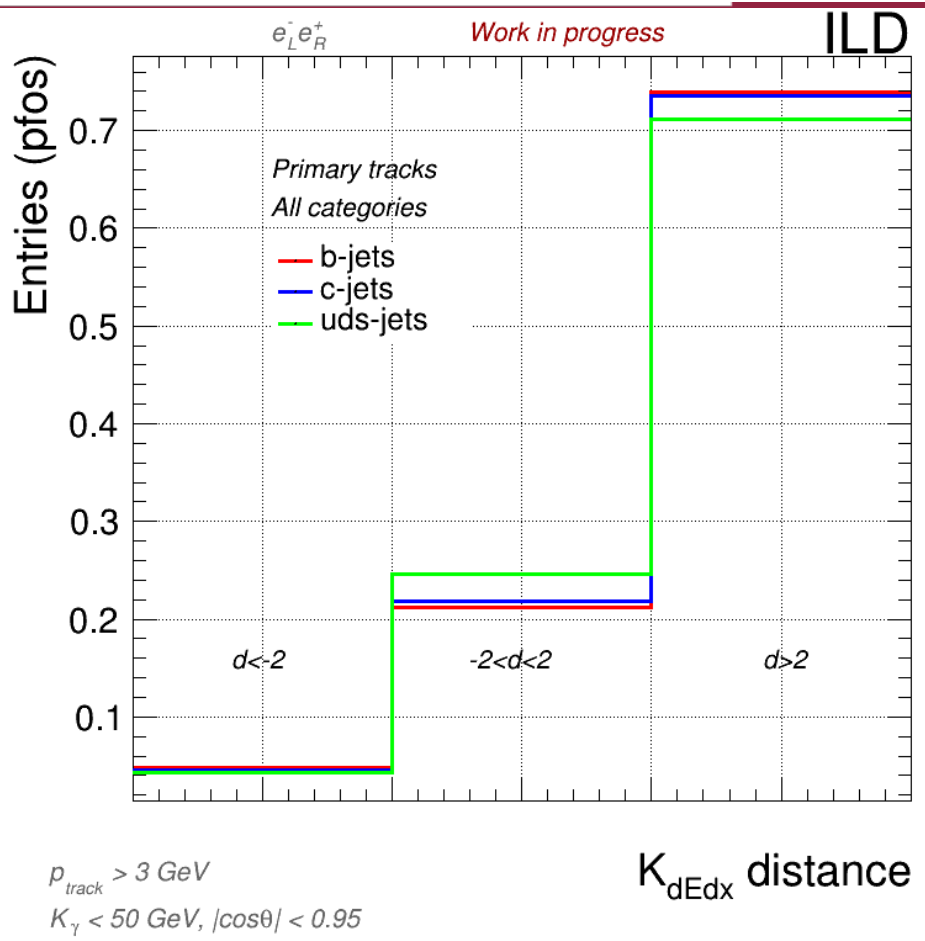
Jet by Jet!

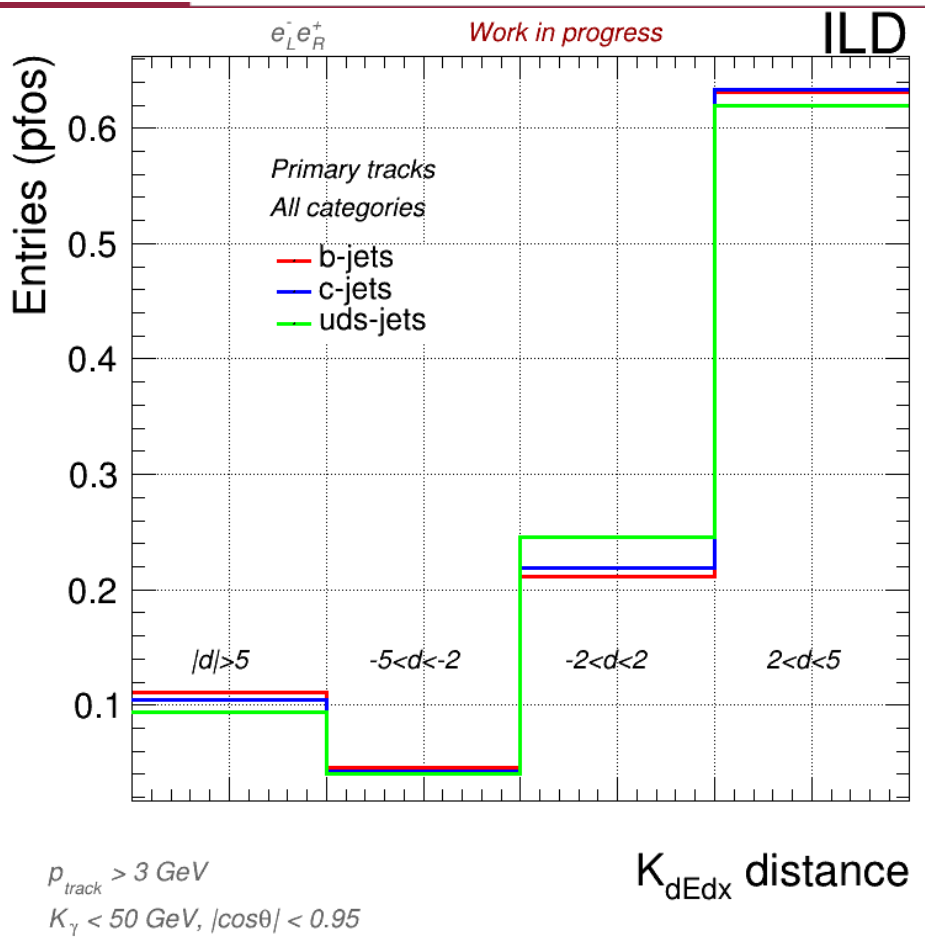
dEdx – KDS for different quark flavours



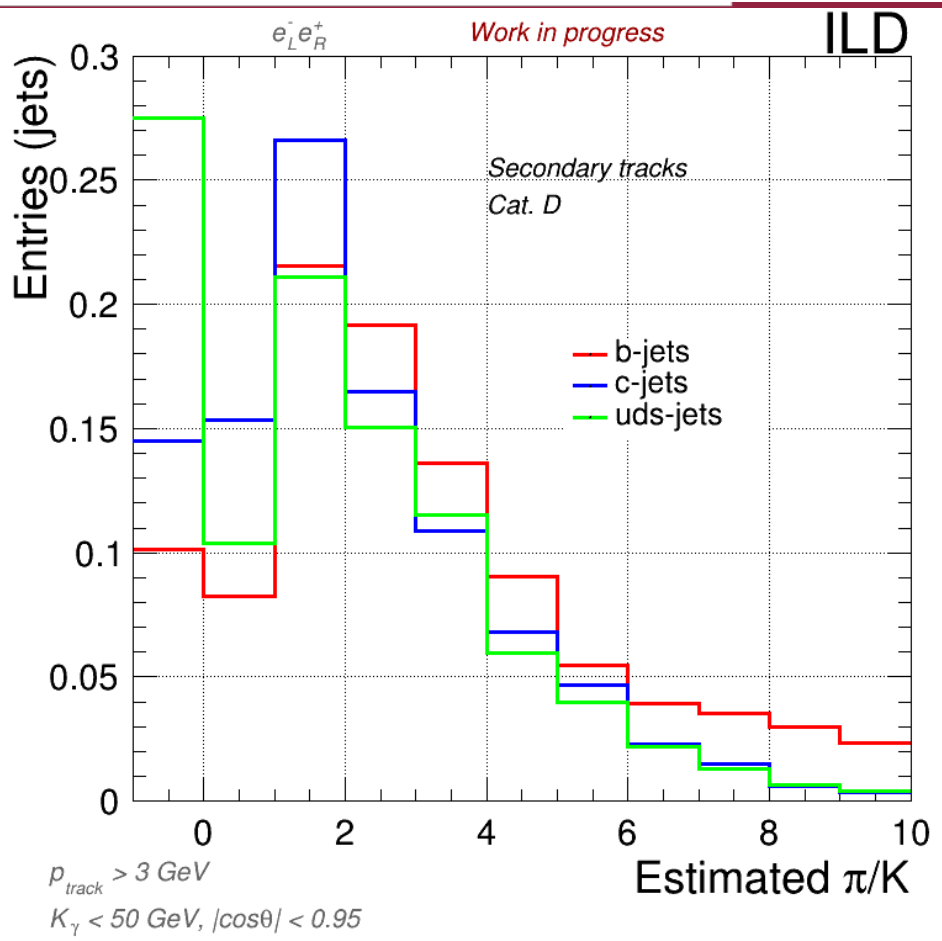


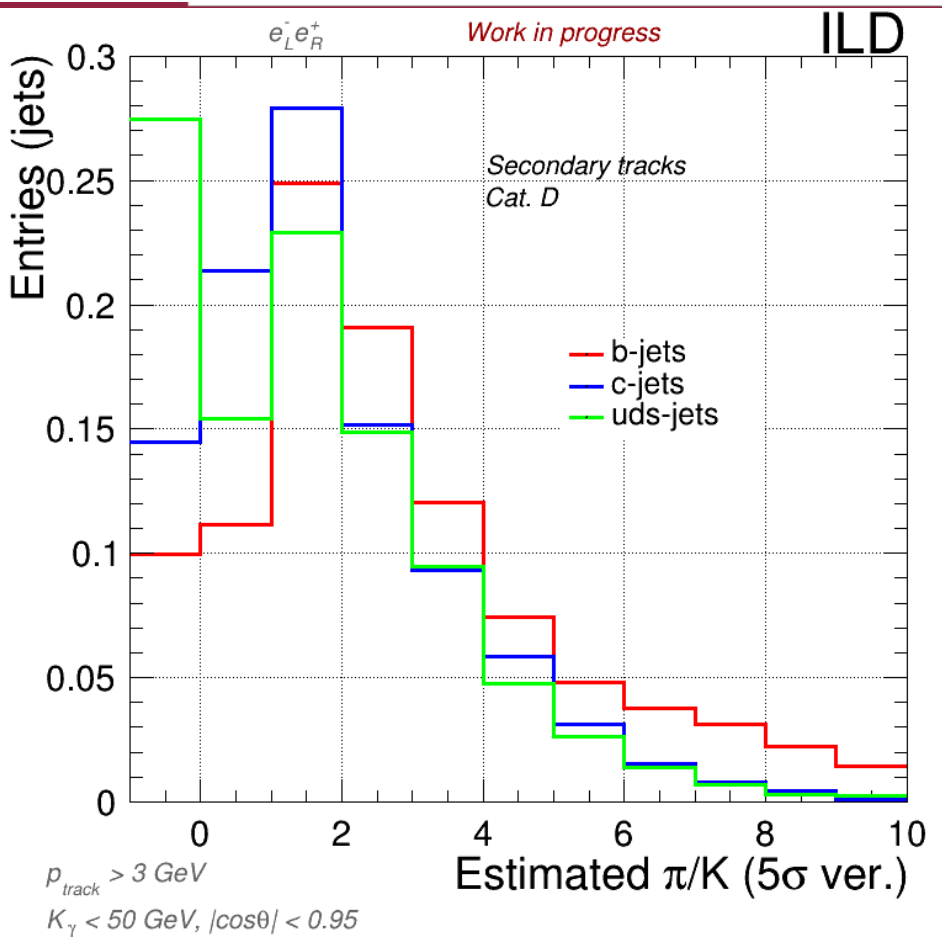
dEdx – KDS classification





dEdx – KDS classification comparison





The "5σ version" seems to work slightly better

dEdx – Next moves

- Now that we have checked these variables it's time to implement them to LCFI+:
  - We have a total of 6 new variables per category (3 ratios for primary and secondary vertexes).

- Working on it!
  - Trying to implement it following the inner structure of LCFI+ and minimizing incompatibilities.

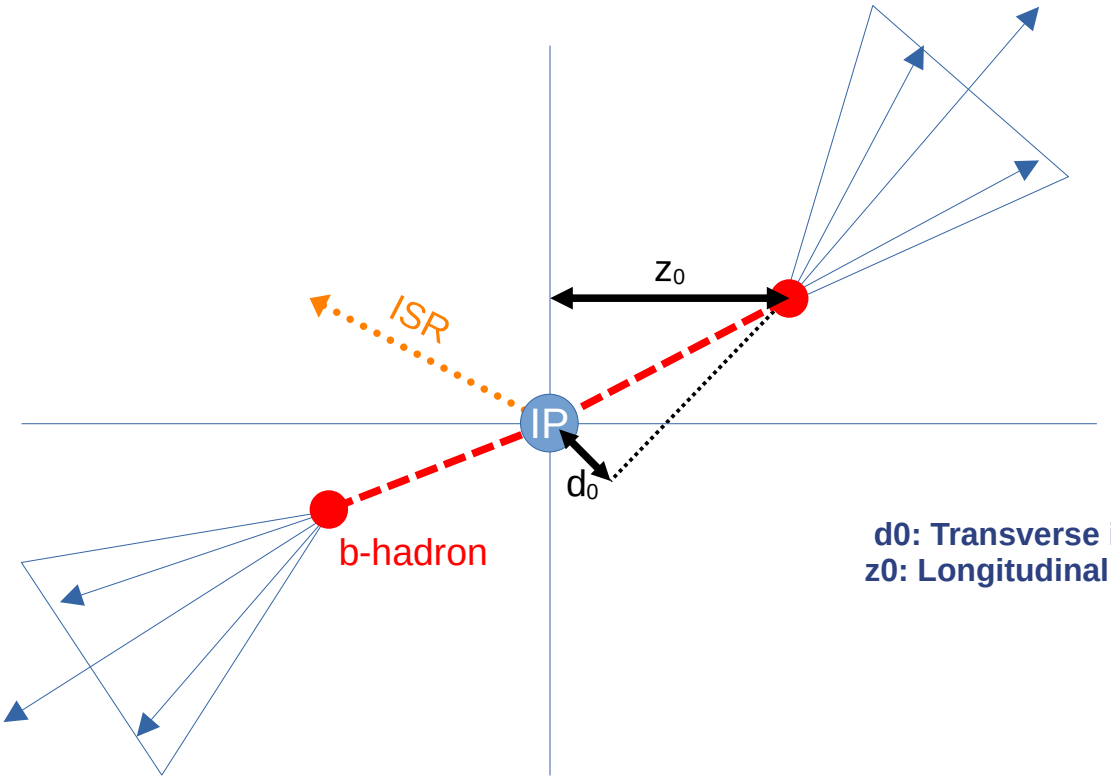
- Once finished:
  - We will check the impact on these parameters in the PFO optimised weights.

Working in progress!

Thanks for your attention!

Back-up

LCFI+ (impact parameters)



d0: Transverse impact parameter
z0: Longitudinal impact parameter

Events for each category

Without ISR removal

Z-Pole (LCFI+ paper[1])

Events (%)			
Cat.	b jets	c jets	uds jets
A	22.9	59.5	98.1
B	39.7	39.8	1.80
C	13.5	0.54	0.02
D	23.8	0.19	0.04

1. LCFIPlus: A Framework for Jet Analysis in Linear Collider Studies

250 GeV samples

Events (%)			
Cat.	b jets	c jets	uds jets
A	20.8	50.8	98.0
B	28.4	46.6	1.59
C	21.7	1.98	0.13
D	29.1	0.59	0.25

500 GeV samples

Events (%)			
Cat.	b jets	c jets	uds jets
A	18.3	45.6	96.3
B	28.0	49.0	2.82
C	21.3	3.84	0.29
D	32.4	1.52	0.59

Category	A	B	C	D
Number of vertices	0	1	1	2
Number of single-track pseudovertices	0-2	0	1	0

Events for each category

With ISR removal

Z-Pole (LCFI+ paper[1])

Events (%)			
Cat.	b jets	c jets	uds jets
A	22.9	59.5	98.1
B	39.7	39.8	1.80
C	13.5	0.54	0.02
D	23.8	0.19	0.04

1. LCFIPlus: A Framework for Jet Analysis in Linear Collider Studies

250 GeV samples

Events (%)			
Cat.	b jets	c jets	uds jets
A	13.9	46.2	98.2
B	30.5	51.0	1.59
C	23.9	2.29	0.11
D	31.7	0.55	0.14

500 GeV samples

Events (%)			
Cat.	b jets	c jets	uds jets
A	11.2	35.8	96.7
B	28.6	58.3	2.64
C	22.9	4.65	0.26
D	37.3	1.27	0.42

Category	A	B	C	D
Number of vertices	0	1	1	2
Number of single-track pseudovertices	0-2	0	1	0

TMVA in LCFI+ (variables)

Name	Description	Normalization factor	Used by category
trk1d0sig	d0 significance of track with highest d0 significance	1	A, B, C, D
trk2d0sig	d0 significance of track with second highest d0 significance	1	A, B, C, D
trk1z0sig	z0 significance of track with highest d0 significance	1	A, B, C, D
trk2z0sig	z0 significance of track with second highest d0 significance	1	A, B, C, D
trk1pt	transverse momentum of track with highest d0 significance	$1/E_{\text{jet}}$	A, B, C, D
trk2pt	transverse momentum of track with second highest d0 significance	$1/E_{\text{jet}}$	A, B, C, D
jprobr	joint probability in the r-phi plane using all tracks	1	A, B, C, D
jprobr5sigma	joint probability in the r-phi plane using all tracks having impact parameter significance exceeding 5 sigma	1	A, B, C, D
jprobz	joint probability in the z projection using all tracks	1	A, B, C, D
jprobz5sigma	joint probability in the z projection using all tracks having impact parameter significance exceeding 5 sigma	1	A, B, C, D
d0bprob	product of b-quark probabilities of d0 values for all tracks, using b/c/q d0 distributions	1	A, B, C, D
d0cprob	product of c-quark probabilities of d0 values for all tracks, using b/c/q d0 distributions	1	A, B, C, D
d0qprob	product of q-quark probabilities of d0 values for all tracks, using b/c/q d0 distributions	1	A, B, C, D
z0bprob	product of b-quark probabilities of z0 values for all tracks, using b/c/q z0 distributions	1	A, B, C, D
z0cprob	product of c-quark probabilities of z0 values for all tracks, using b/c/q z0 distributions	1	A, B, C, D
z0qprob	product of q-quark probabilities of z0 values for all tracks, using b/c/q z0 distributions	1	A, B, C, D
nmuon	number of identified muons	1	A, B, C, D
nelectron	number of identified electrons	1	A, B, C, D
trkmass	mass of all tracks exceeding 5 sigma significance in d0/z0 values	1	A, B, C, D

TMVA in LCFI+ (variables)

Name	Description	Normalization factor	Used by category
1vtxprob	vertex probability with all tracks associated in vertices combined	1	B, C, D
vtxlen1	decay length of the first vertex in the jet (zero if no vertex is found)	$1/E_{\text{jet}}$	B, C, D
vtxlen2	decay length of the second vertex in the jet (zero if number of vertex is less than two)	$1/E_{\text{jet}}$	D
vtxlen12	distance between the first and second vertex (zero if number of vertex is less than two)	$1/E_{\text{jet}}$	D
vtxsig1	decay length significance of the first vertex in the jet (zero if no vertex is found)	$1/E_{\text{jet}}$	B, C, D
vtxsig2	decay length significance of the second vertex in the jet (zero if number of vertex is less than two)	$1/E_{\text{jet}}$	D
vtxsig12	vtxlen12 divided by its error as computed from the sum of the covariance matrix of the first and second vertices, projected along the line connecting the two vertices	$1/E_{\text{jet}}$	D
vtxdirang1	the angle between the momentum (computed as a vector sum of track momenta) and the displacement of the first vertex	E_{jet}	B, C, D
vtxdirang2	the angle between the momentum (computed as a vector sum of track momenta) and the displacement of the second vertex	E_{jet}	D
vtxmult1	number of tracks included in the first vertex (zero if no vertex is found)	1	B, C, D
vtxmult2	number of tracks included in the second vertex (zero if number of vertex is less than two)	1	D
vtxmult	number of tracks which are used to form secondary vertices (summed for all vertices)	1	D
vtxmom1	magnitude of the vector sum of the momenta of all tracks combined into the first vertex	$1/E_{\text{jet}}$	B, C, D
vtxmom2	magnitude of the vector sum of the momenta of all tracks combined into the second vertex	$1/E_{\text{jet}}$	D
vtxmass1	mass of the first vertex computed from the sum of track four-momenta	1	B, C, D
vtxmass2	mass of the second vertex computed from the sum of track four-momenta	1	D
vtxmass	vertex mass as computed from the sum of four momenta of all tracks forming secondary vertices	1	B, C, D
vtxmasspc	mass of the vertex with minimum pt correction allowed by the error matrices of the primary and secondary vertices	1	B, C, D
vtxprob	vertex probability; for multiple vertices, the probability P is computed as 1-P = (1-P1)(1-P2)...(1-PN)	1	B, C, D

Boosted Decision Trees (BDT) - Overview

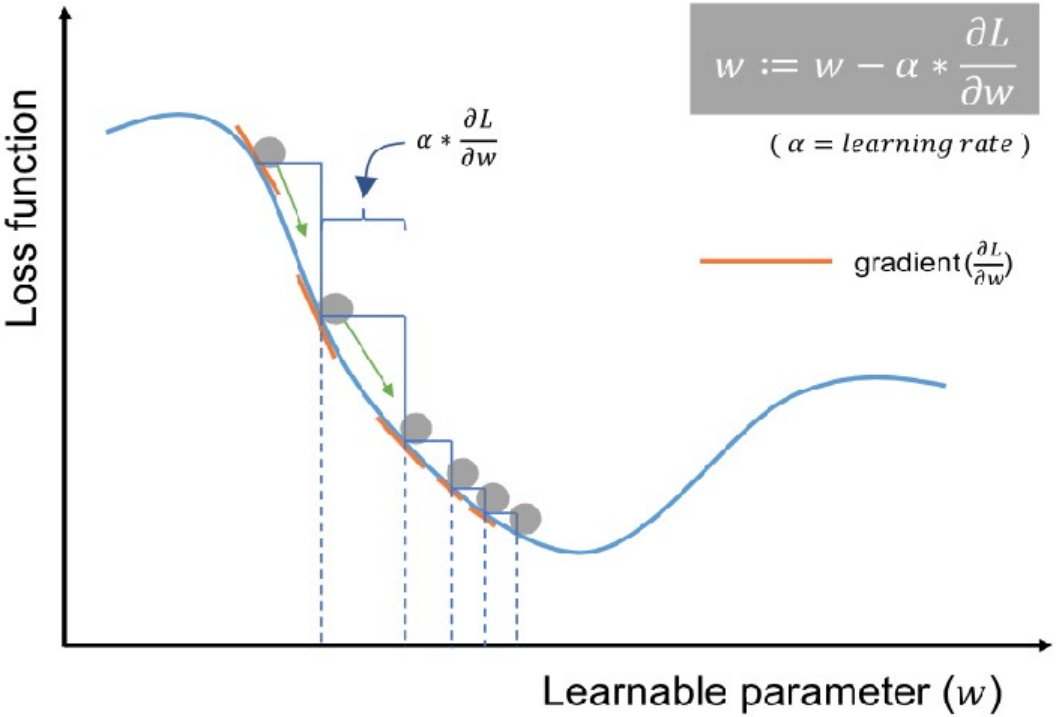
- A decision tree is a weak learner (an estimator): It classifies your data according to certain/s question/s (nº of leaves).
- Boosting is using many of these trees one after each other until you get a final classification.
  - Gradient Boosting is the most common one (and the one I'm using):

$$F_m(x) = F_{m-1}(x) + \eta \cdot h_m(x),\ 0 < \eta \leq 1$$

    - Where F is the total prediction, h the prediction of a tree, and η is the learning rate (or **shrinkage**).
      - Each of the trees actually perform its classification using the gradient of the loss function of the previous one, so it keeps "refining" the result.

Boosted Decision Trees (BDT) - Overview

- Simple visual representation[1]:



1. Website (Bradley Boehmke & Brandon Greenwell): https://bradleyboehmke.github.io/HOML/gbm.html

PSO – Implementation - Origin

- I didn't start from scratch, but rather adapted Andrej Saibel's code. This code:
  - Is a signal-background classifier (2 classes).
    - Uses ROOT's classes that are optimal to Signal-vs-Background classifiers.
  - Includes nTuples variables as extra parameters to play with.
    - Optimizes the use of physical variables as well.
  - Includes a test to avoid overfitting (Kolmogorov-Smirnoff test).
  - Includes different types of FOM to choose from.
  - Was originally prepared to run in CMS computing services.
    - There are different codes interacting in Python, C (C++) and bash; to prepare the particles, executing them, read the results and update their new configurations.

PSO – Kolmogorov-Smirnov Test

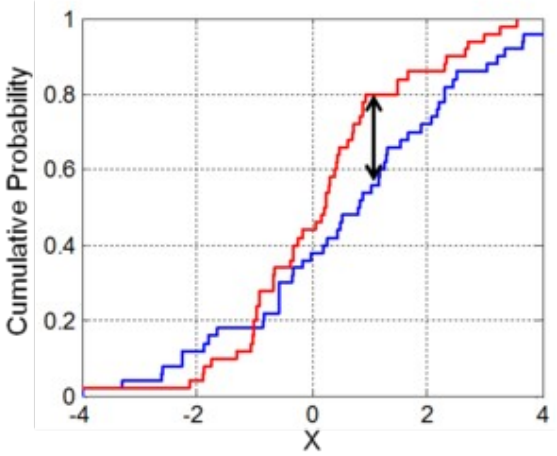
- Compare how likely there is that two different empirical distributions (histograms) came from the same underlying distribution function.
  - It uses the max. distance between the cumulative probability(CPD) of both histograms:

$$D_{n,m} = \sup_x |F_{1,n}(x) - F_{2,m}(x)|$$

  - Then, we past a test for such distance to a certain degree of significance level α (usually 0.05):

$$D_{n,m} > \sqrt{-\ln\left(\frac{\alpha}{2}\right) \cdot \frac{1+\frac{m}{n}}{2m}}.$$

  - The output is a p-value which determine how likely it is that both histograms came from the same distribution according to our significance level (e.g. 0.05 stands for 95% of agreement).



Notice how a big jump in the CPD even in a very narrow region will lead to a very high distance (low KS score): Hyper-sensibility if the distributions are not smooth enough

PSO – Anderson-Darling Test

- The AD test statistic is defined as:

$$A^2 = -n - S$$

- Where:

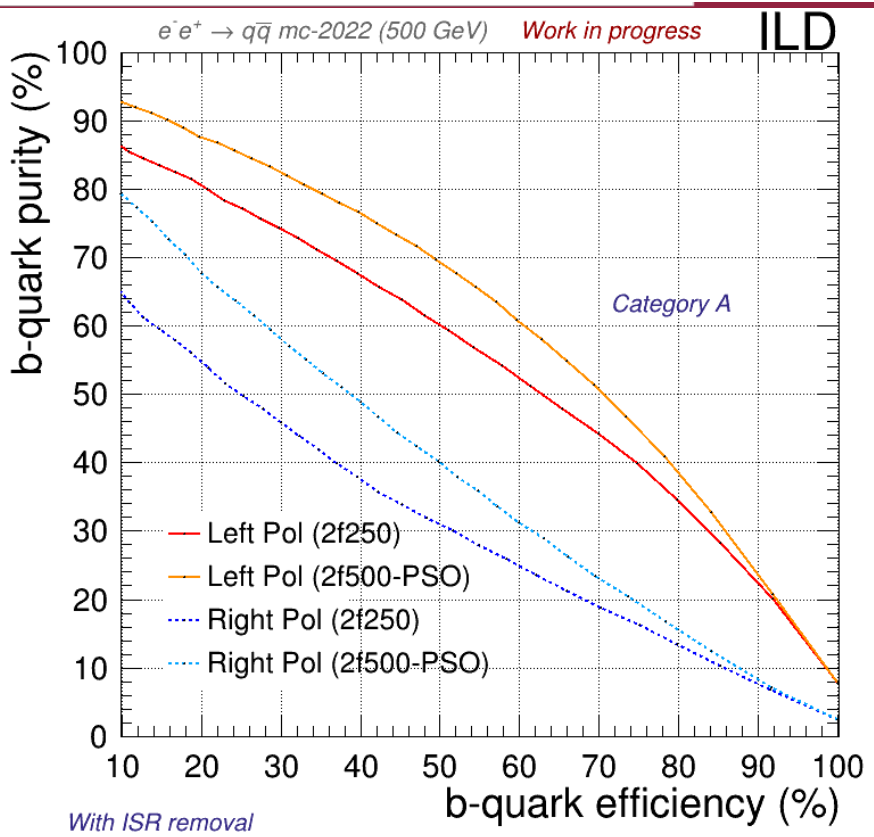
$$S = \sum_{i=1}^{n} \frac{2i-1}{n} \left[\ln(F(Y_i)) + \ln(1 - F(Y_{n+1-i}))\right]$$

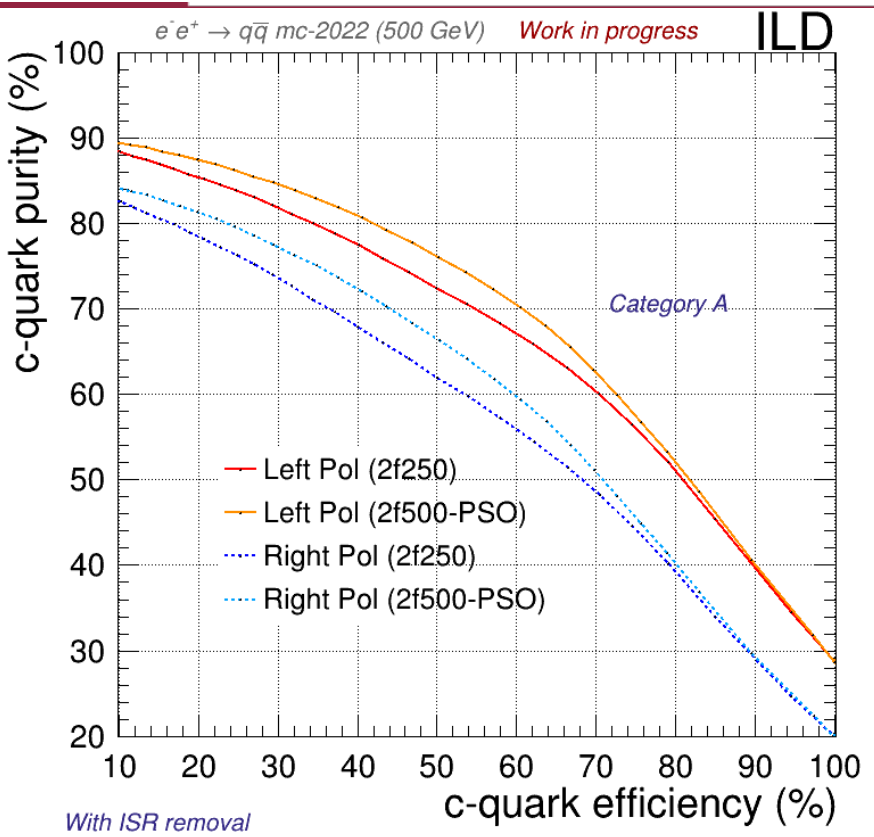
- Being F the cumulative probability distribution for a certain distribution (or the other sample in our 2-samples scenario).
  - Works better with uniform distributions and higher binning.
- Again, the output is an estimator based on a cut in $A > A_{critical}$

Notice how this kind of testing avoid the hyper-sensibility that we had in narrow jumps in the CPD but what if one of these jumps in CPD is actually relevant?

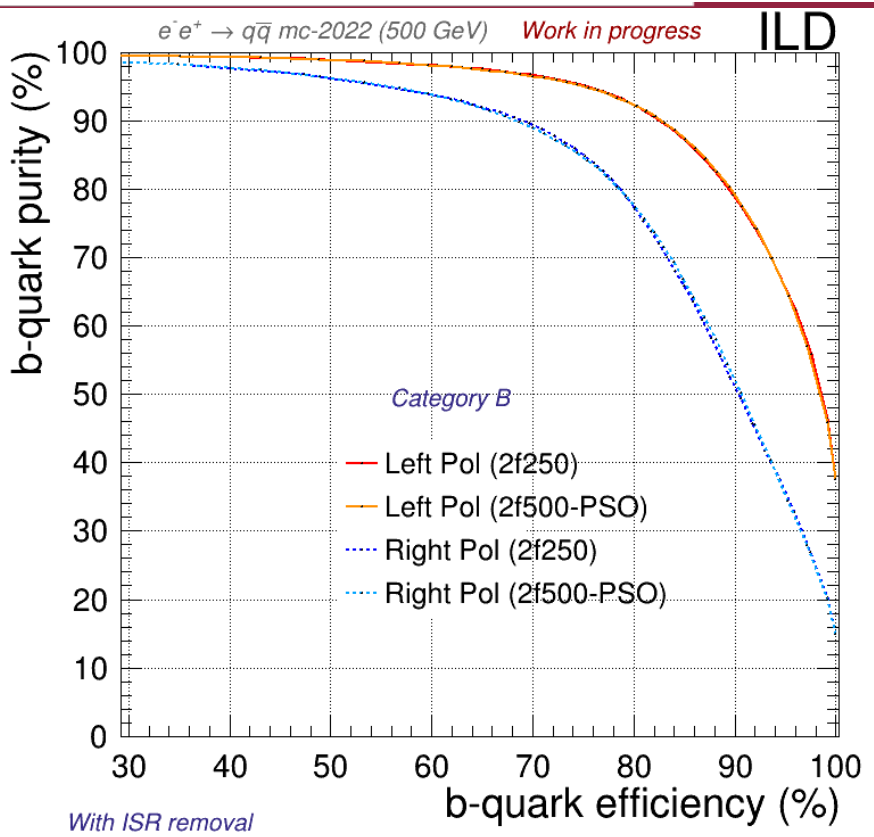
I chose very conservative (and secure) way to proceed: Applying both tests!

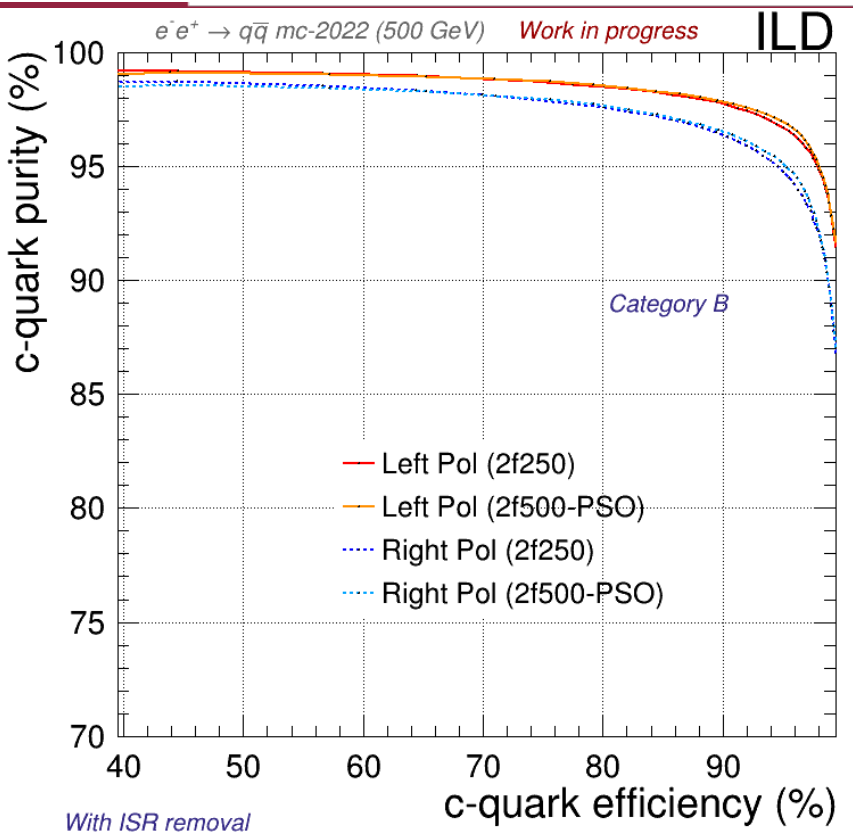
PSO Performance (500 GeV) – Cat. A



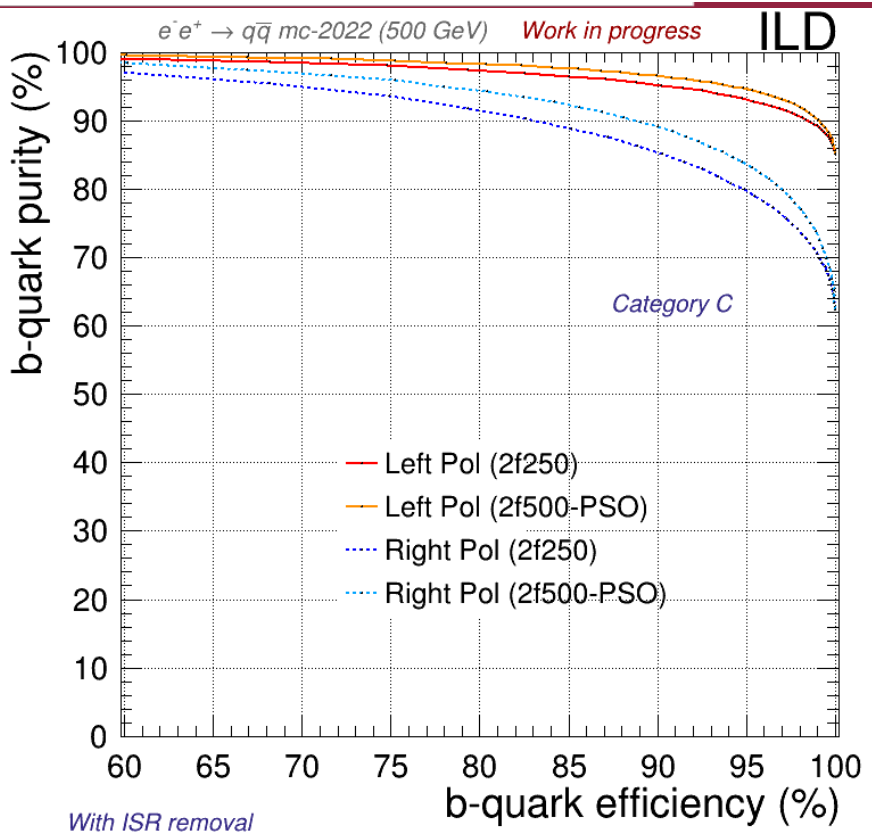


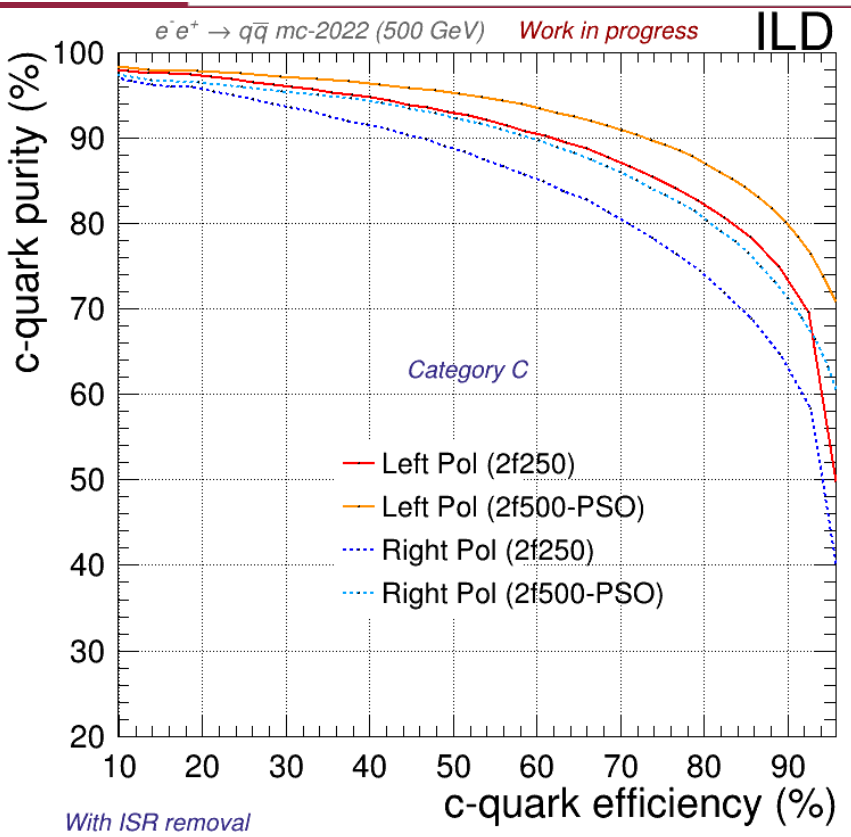
PSO Performance (500 GeV) – Cat. B



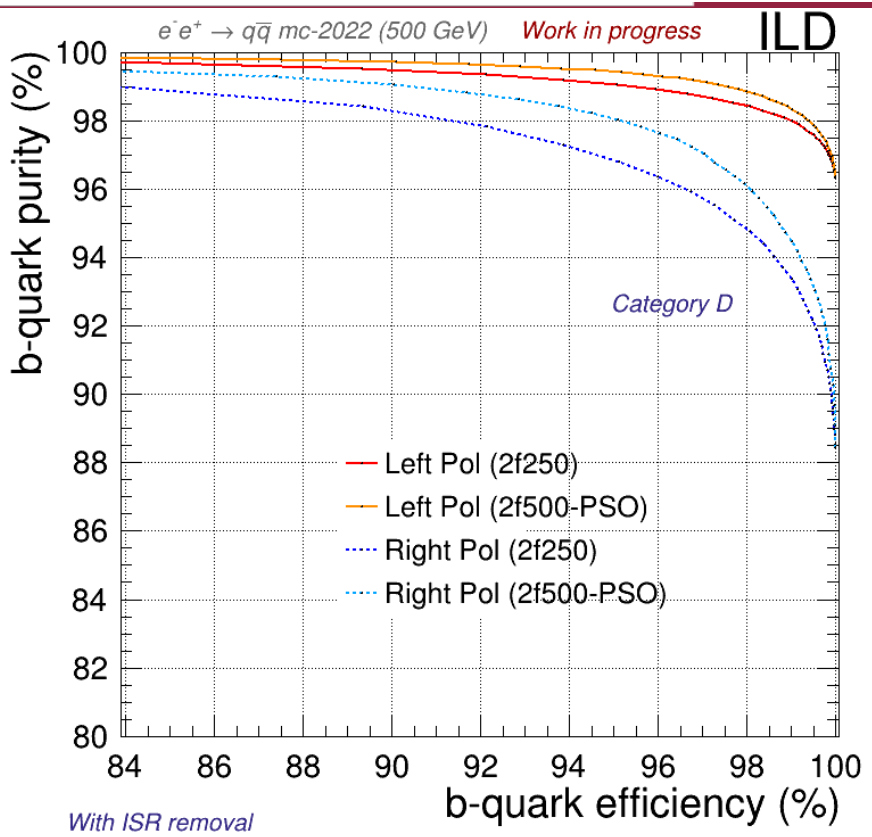


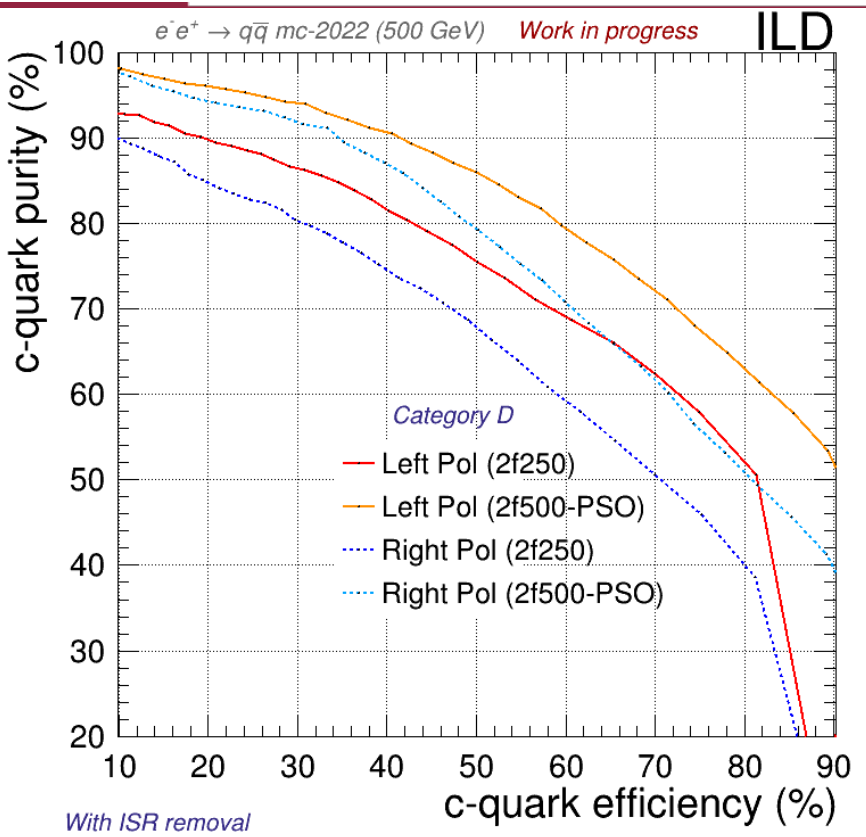
PSO Performance (500 GeV) – Cat. C



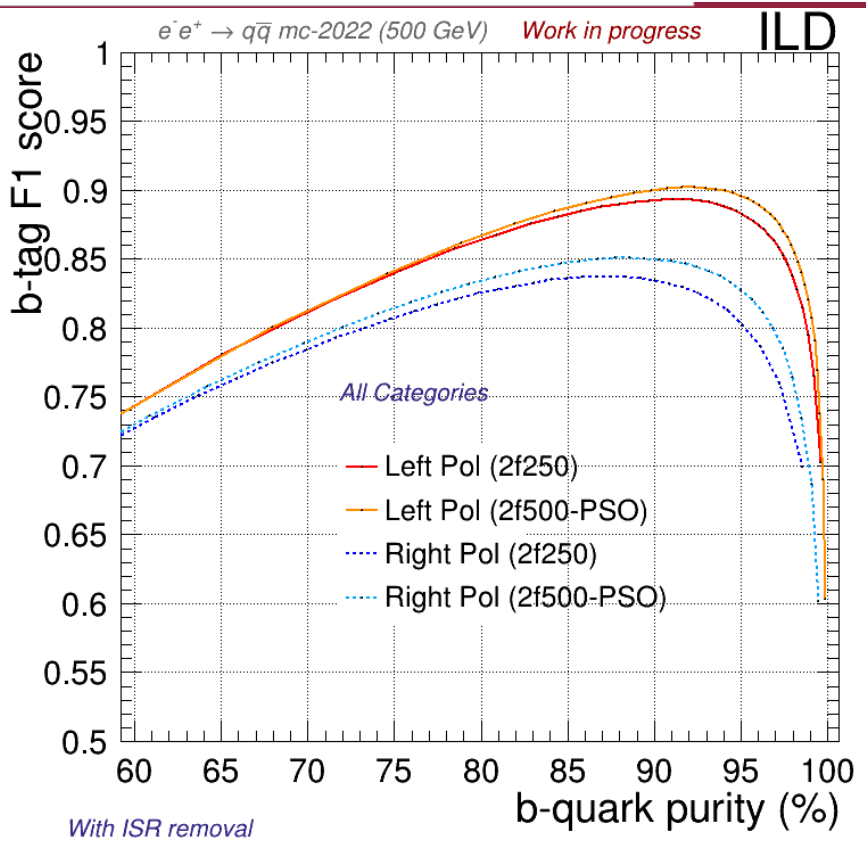


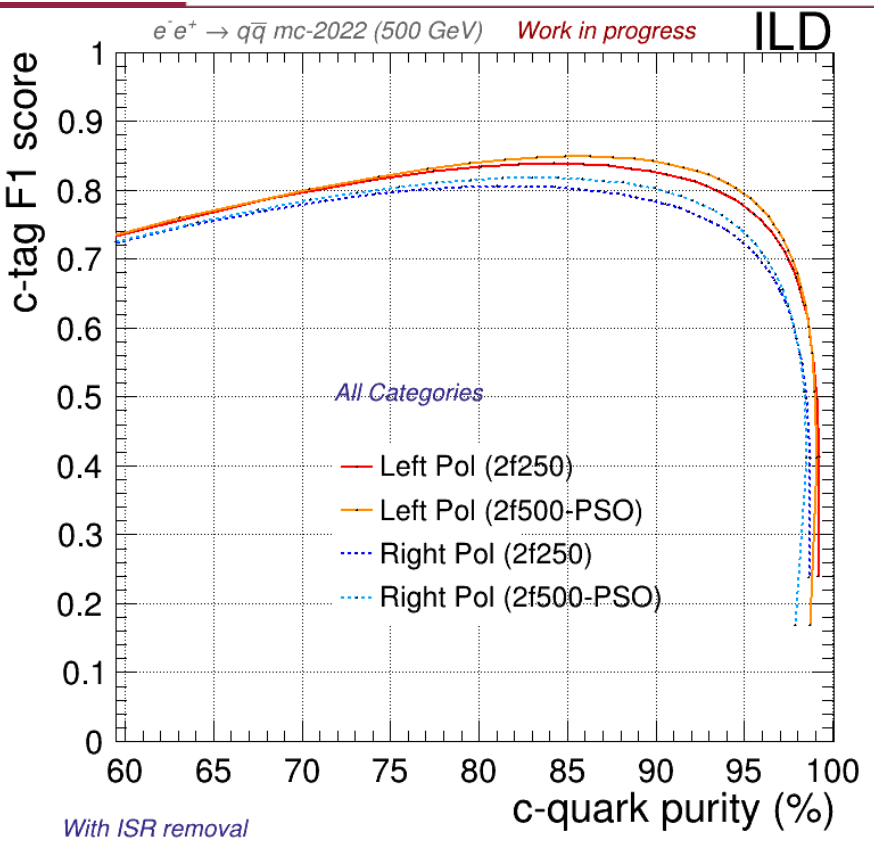
PSO Performance (500 GeV) – Cat. D





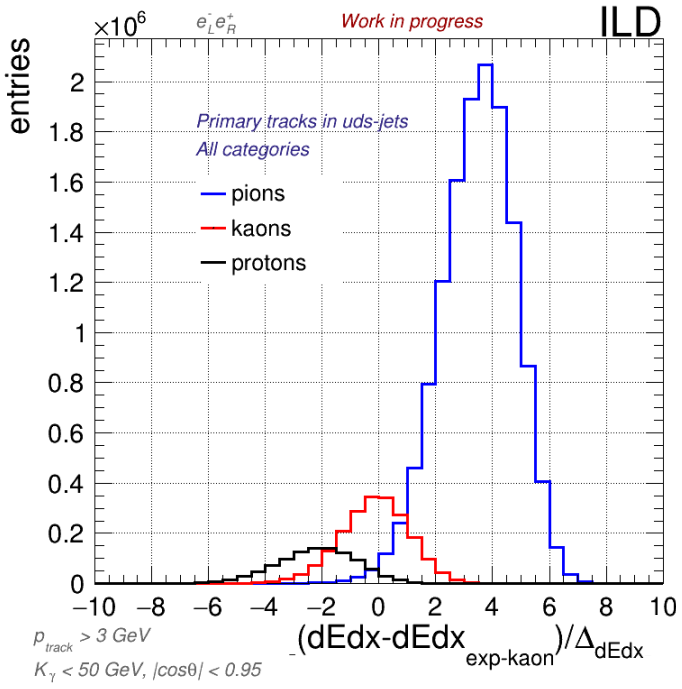
F1 score & maximum purity (500 GeV)

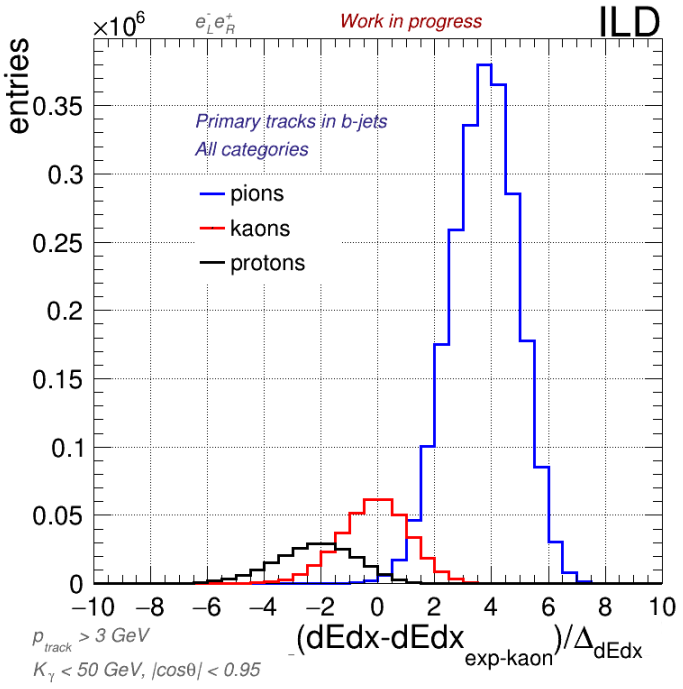


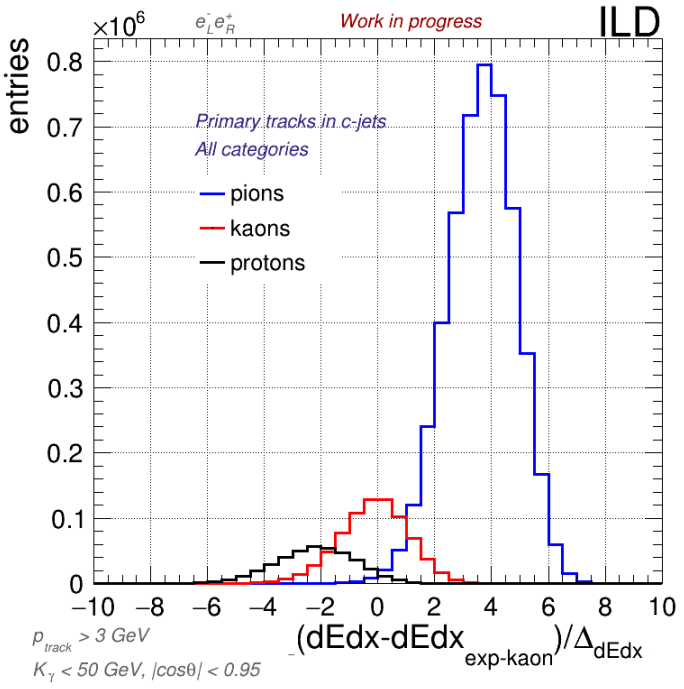


$$F_1 = \frac{tp}{tp + \frac{1}{2}(fp + fn)}$$

Using dEdx for flavour tagging

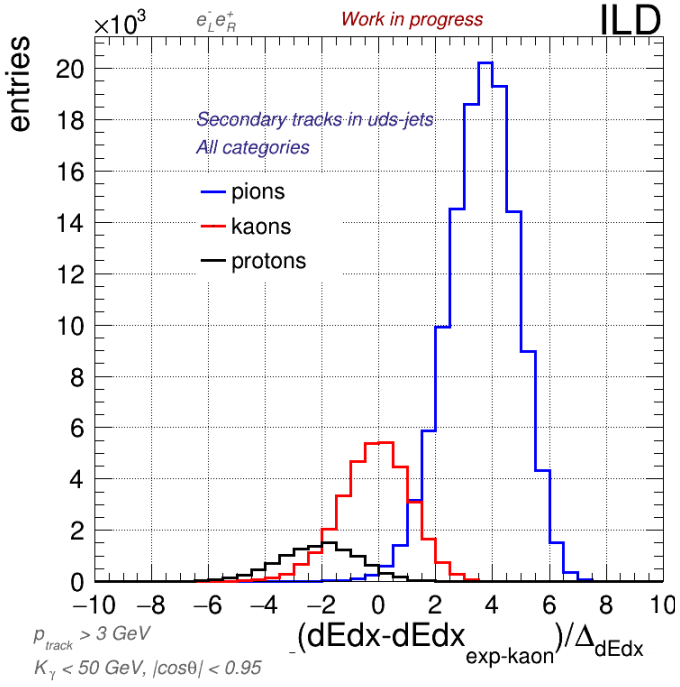


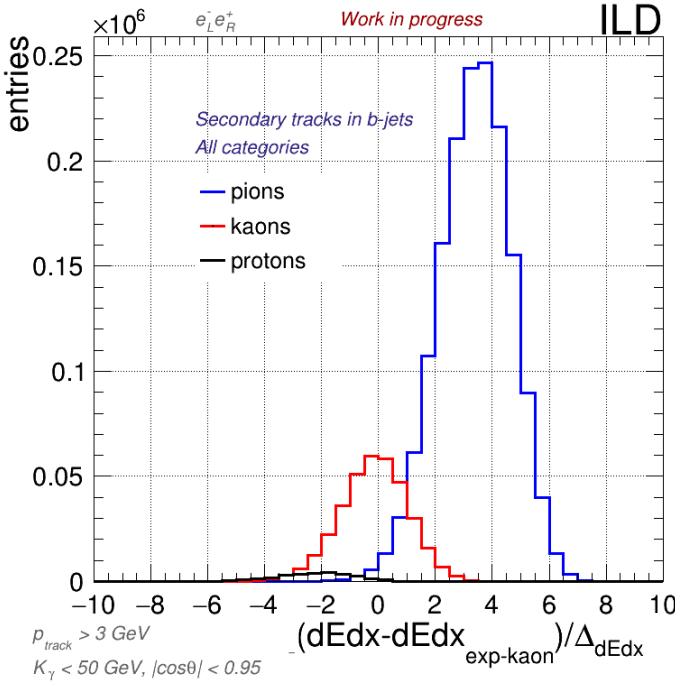


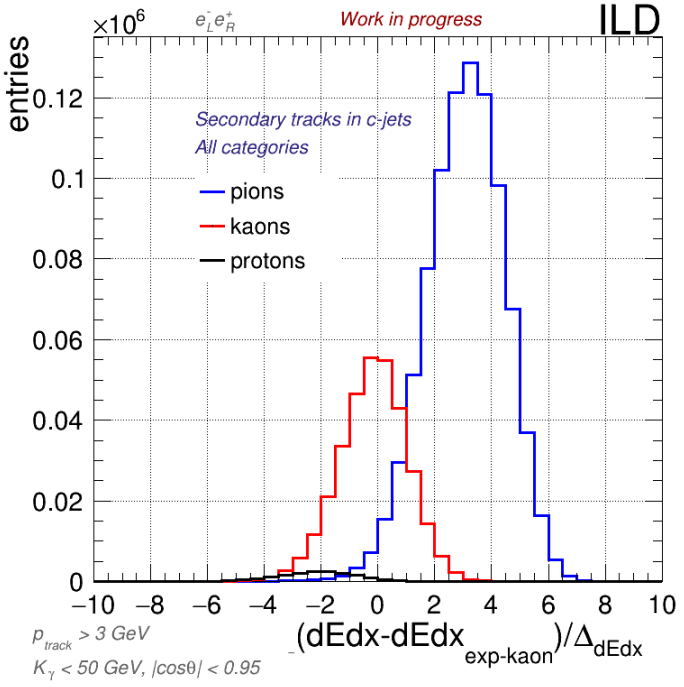


We differentiate between primary & secondary tracks

Using dEdx for flavour tagging

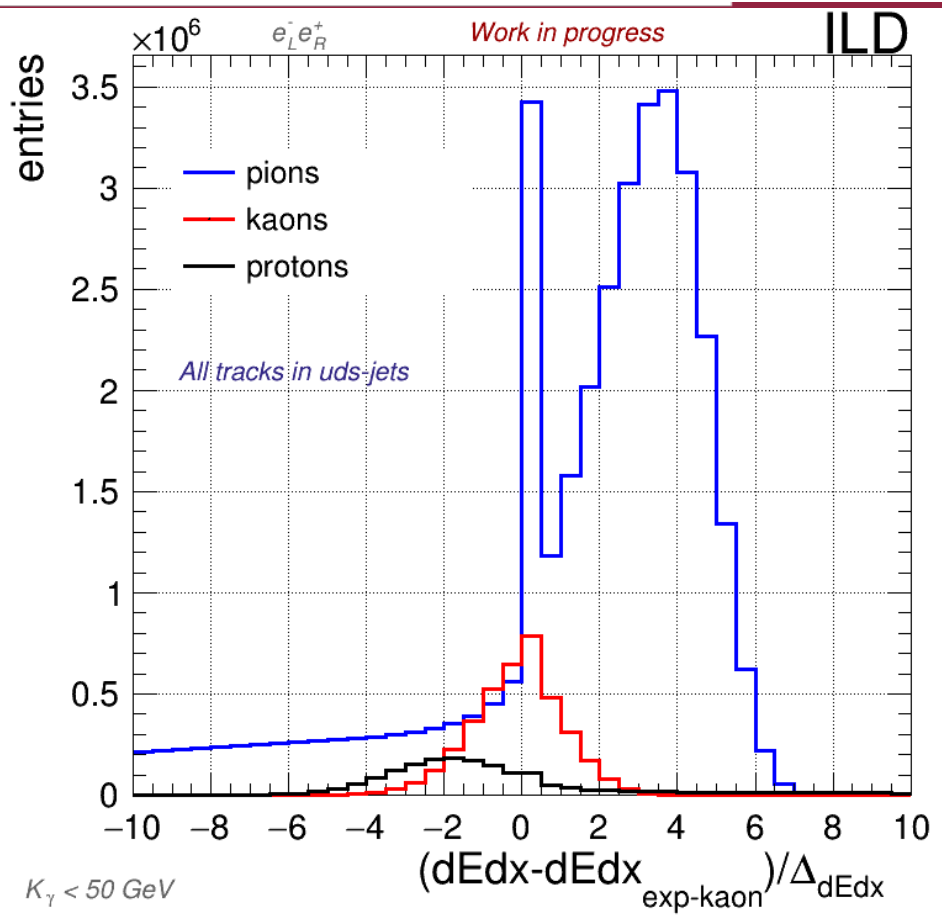


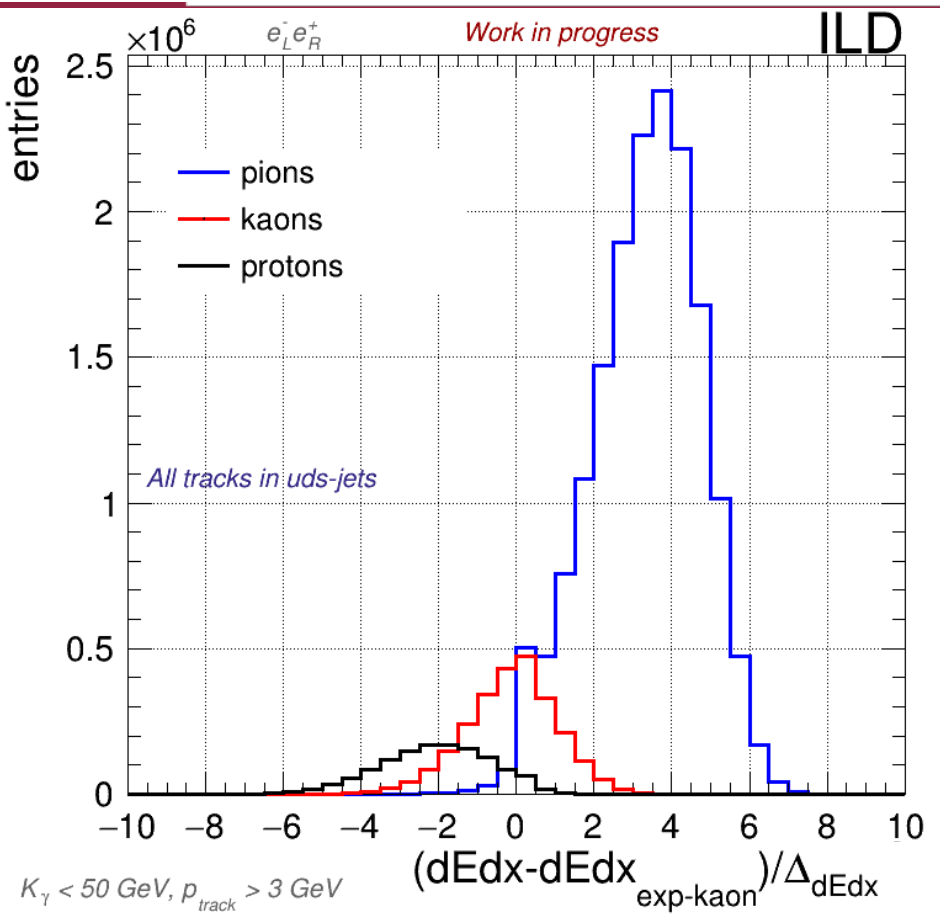




We differentiate between primary & secondary tracks

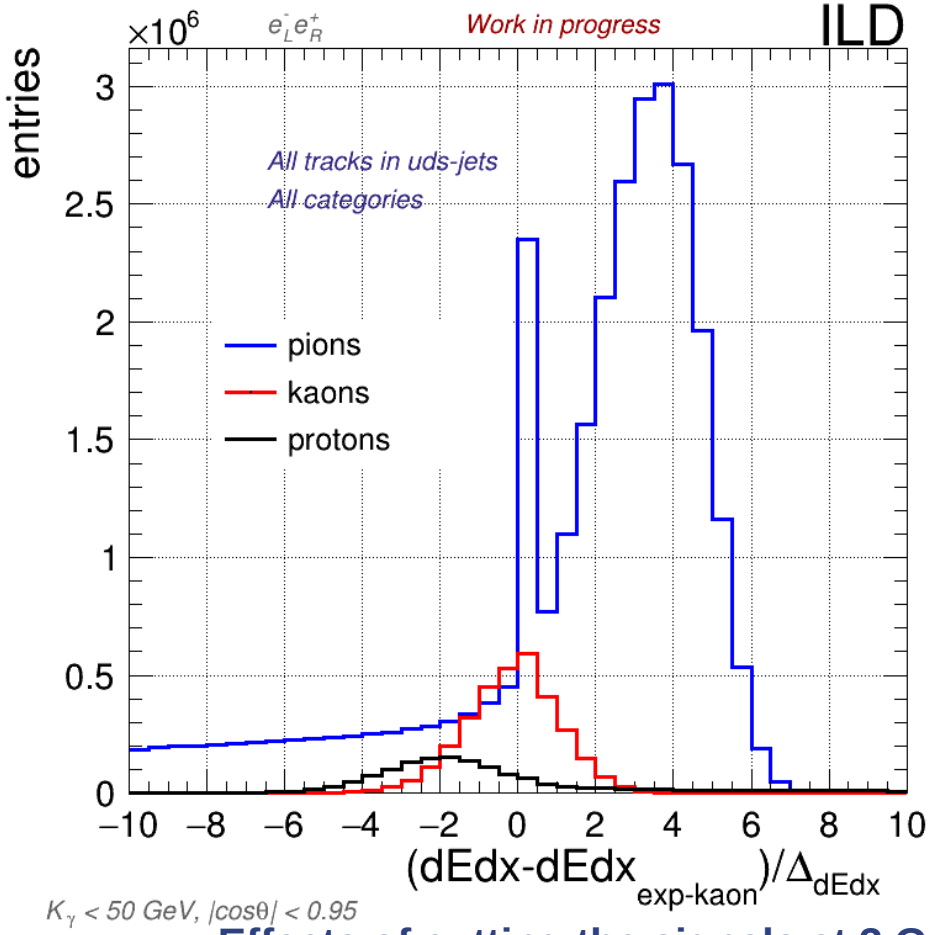
Using dEdx for flavour tagging

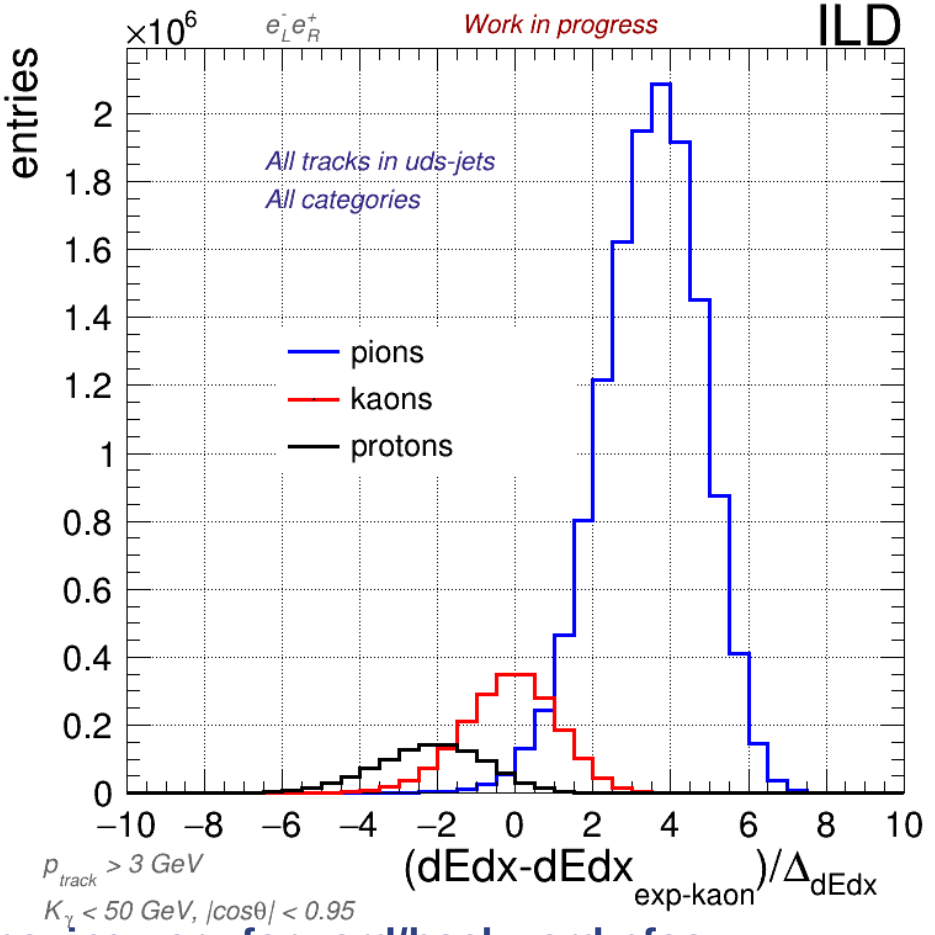




Effects of cutting the signals at 3 GeV, first attempt

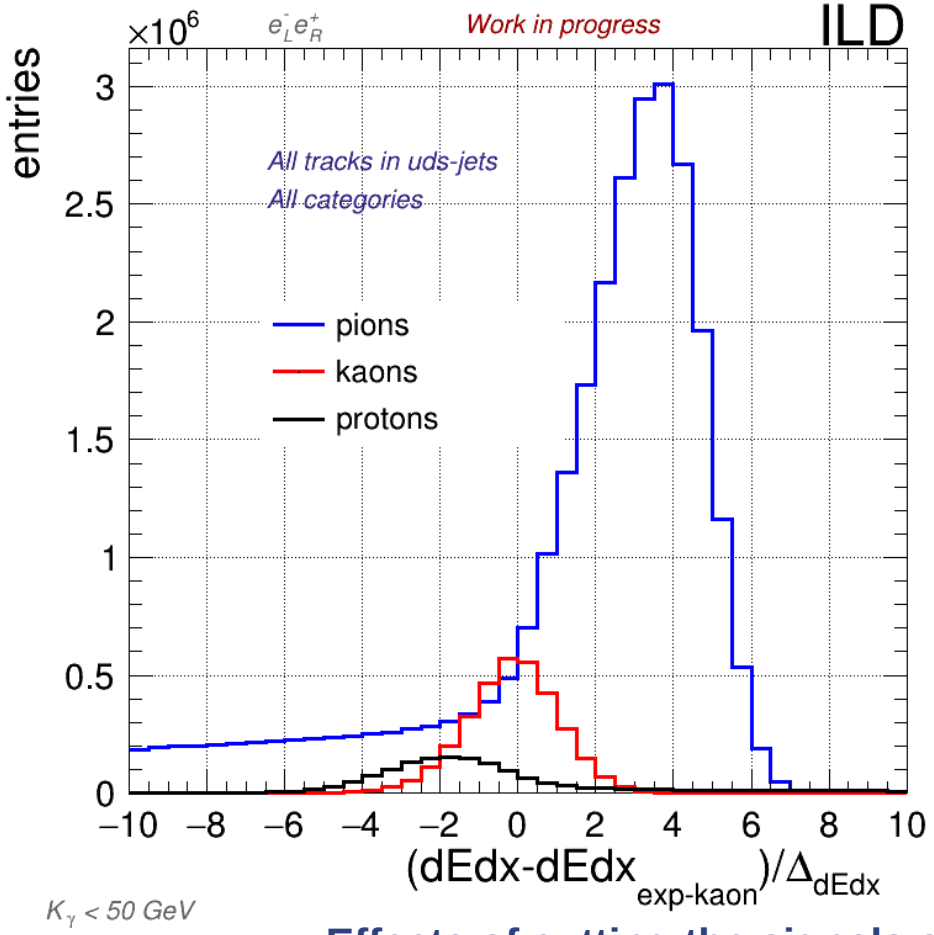
Using dEdx for flavour tagging

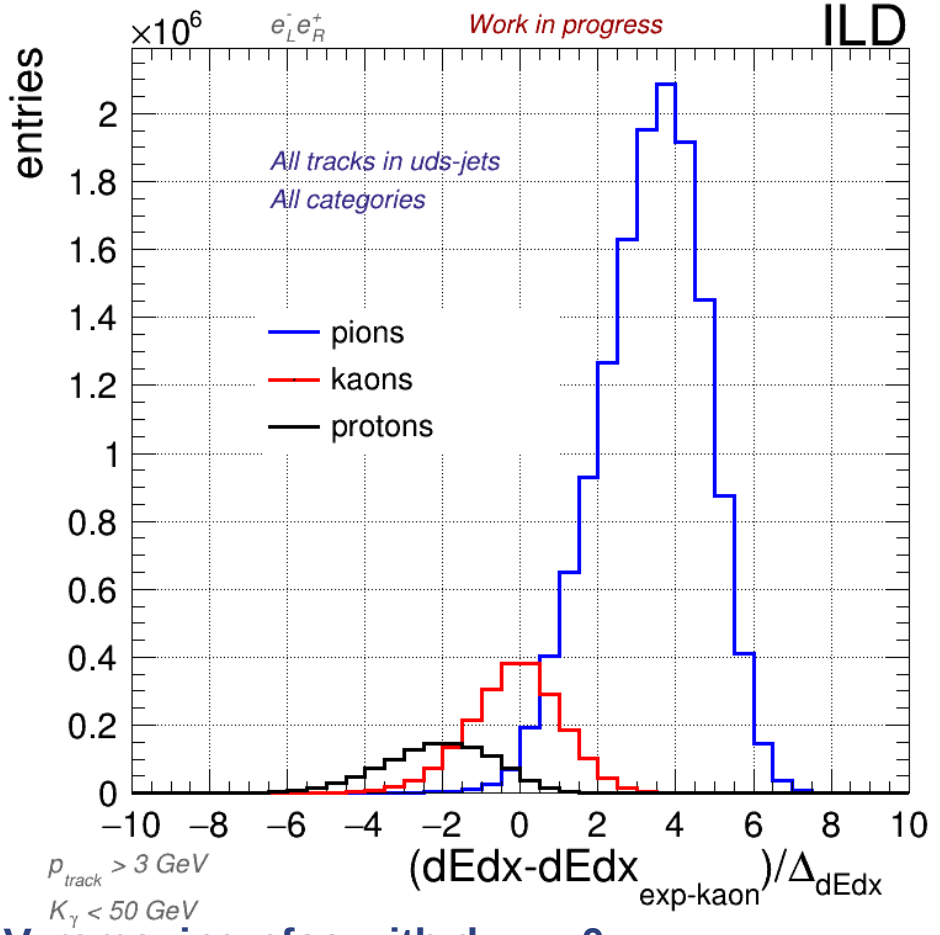




Effects of cutting the signals at 3 GeV, removing very forward/backward pfos

Using dEdx for flavour tagging





Effects of cutting the signals at 3 GeV, removing pfos with $d_{kaon} = 0$

Probably an initialization issue (in *dEdxKaonDistance*)